

Automated exploration of the conformational degrees of freedom along reaction profiles - driving a FASTCAR

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1 RSMD threshold - additional elements

In order to highlight the adequacy of the chosen RMSD threshold, we conducted additional test calculations in the case of the major reaction pathway in the organocatalysed Black rearrangement. We opted here for a CREST search using a solvent model (CH₂Cl₂, only available in CREST with a similar polarity to that of 2-methyl-2-propanol) with default parameters, a cregen

pruning with an energy window of 30 kcal/mol (default parameter in FASTCAR), and with variable RMSD thresholds: 0.0, 0.3, 0.5 and 0.7. The same starting transition state structure was used in all cases (first structure in subsection 4.1).

The CREST analysis resulted in this case in 23 proposed structures, reducing to 21 candidates after cregen. We list in Table 1 the number of unique, duplicate and "garbage" structures reported after each FASTCAR run, along with the energy of the lowest transition state structure and the energy span covered by the TS structures.

RMSD value	U.	D.	G.	E_{min}
0.0	7	2	11	-1488.75261373
0.3	5	3	4	-1488.75261367
0.5	6	1	3	-1488.75261370
0.7	4	0	2	-1488.75261373

Table 1: Impact of the RMSD threshold on the number of unique (U.), duplicate (D.) and garbage (G.) TS structures. In all cases the energy of the lowest TS structures is given, in atomic units.

When the RMSD threshold is set to zero (all structures considered), one may note that the major consequence is an explosion in the number of garbage structures (non TS or not converging): most of the computational effort at the DFT level is "lost" on irrelevant geometries. As one may note, the lowest energy structure is in any case always located, which suggests that - at least in this case - the RMSD cut-off does not alter the location of the lowest energy TS structure.

On the other hand, the variation in the total number of structures (from 7 to 4) indicates that the RMSD cut-off may alter the coverage of the intermediate energy landscape. We list in Table 2 the relative energies of the recovered structures in the 4 runs, identifying the structures to their number in the RMSD=0 case.

As one can see from this, the energy window spanned by the TS structure is the same when the RMSD threshold is set to 0.3, 0.5 and 0.7. The missing structures are in fact here found at intermediate energies, which implies the RMSD cut-off is likely to alter conclusions drawn from an ensemble analysis (*e.g.* Maxwell-Boltzmann statistical analysis). At 0.7, two low-energy structures (0.6 and 1.4 kcal/mol) are missed, hence the error is expected large. At

0.5, one may note that all relevant structures are identified. More surprising is the disappearance of structure number 4 at RMSD=0.3. A detailed analysis of the ensemble of structures produced by CREST reveals that the two ensembles are not exactly equivalent: in the case of the RMSD=0.3 run, structure number 4 was in fact never produced. This result highlights a rather important fact: although CREST consistently predicted the lowest energy conformer, the same is not necessarily true for the list of low-lying structures. When interested in ensemble data, one should thus run several independent jobs (or iterative ones) to ensure no structure is left behind.

Struc.	RMSD=0.7	RMSD=0.5	RMSD=0.3	RMSD=0
1	0.0	0.0	0.0	0.0
2		0.6	0.6	0.6
3		1.4	1.4	1.4
4	1.7	1.7		1.7
5	1.8	1.8	1.8	1.8
6	2.2	2.2	2.2	2.2
7				3.5

Table 2: Relative energies of the unique transition state structures from the FASTCAR runs with varying RMSD. Values in kcal/mol.

2 Computational details

For the sake of clarity, the chosen levels of theory are as follows:

- B3LYP-D3BJ/6-31G(d,p) for the acidic cyclization.
- IEFPCM(2-Methyl-2-Propanol)-B3LYP-D3/6-31G(d,p) for the first refinement step then IEFPCM(2-Methyl-2-Propanol)-B3LYP-D3/6-311++G(d,p) for the second refinement step for the Black rearrangement.
- B3LYP-D3/6-31G(d,p) for the Diels-Alder reaction.
- IEFPCM(dichloroethane)- ω B97wD/6-31++G(d,p) for the first refinement step and IEFPCM(dichloroethane)- ω B97wD/6-311++G(d,p) for the second refinement step for the regioselective intramolecular radical H-atom transfer.

- BP86/SVP for the enantioselective dialkylzinc additions on benzaldehyde.

The names of TSs resulting from FASTCAR are composed as follows: TS + the name of the basis set, if two steps have been selected + the number of the conformers after CREGEN.

3 Acidic intramolecular cyclisation

3.1 Major diastereoisomer

3.1.1 Starting TS first run

TS Input 1

E(RB3LYP) = -1097.26170428 A.U.

First frequency = -247.3758 cm⁻¹

C	-1.7077801642	0.0578261594	0.9295358505
C	-0.4647471826	-0.476297834	1.6906248616
C	-1.6158544338	1.2778598663	0.0018902299
C	-1.0184407984	0.7117233239	-1.3235914153
C	0.4695893229	0.2641170881	-1.2884686817
N	0.7638786945	-0.5235293473	1.1312046886
C	1.249348577	0.3751917742	0.0436595112
H	1.0135078616	0.8874803417	-1.9992266756
H	0.5684041809	-0.7599726639	-1.6614512321
C	1.7604169891	-1.3451747894	1.8525875513
C	2.6457036504	-2.072675256	0.8498963595
H	1.2070155177	-2.038538143	2.4815044463
H	2.3664402202	-0.7043675738	2.5025037104
C	2.722483686	0.1485827031	-0.2715946335
H	1.1680091251	1.4000096435	0.4050240923
C	3.377213682	-1.0531036724	0.0203124404
H	2.0263331973	-2.7329568708	0.2294132337
H	3.3536648626	-2.7091505741	1.3882040802
C	3.4141499294	1.1689179814	-0.9358724837
C	4.7347980595	0.987247662	-1.3368546788
C	5.3811808214	-0.2214757515	-1.0672868583
C	4.7056242616	-1.2276175852	-0.3810774636

H	5.2118334899	-2.1576842688	-0.1389753185
H	6.4119029384	-0.3698491833	-1.372755813
H	2.9164938313	2.113511958	-1.138437813
H	5.2589590676	1.7871016562	-1.8495081288
C	-1.0269470987	2.5459669497	0.6700673033
H	-2.6578983796	1.5201130336	-0.2362551831
H	-0.1869143888	2.263697105	1.314843652
C	-2.0757928639	3.2141149005	1.5710101079
C	-0.5187417488	3.53868128	-0.3837641906
H	-0.1448637388	4.4427919309	0.1038337984
H	-1.3284983741	3.833519541	-1.0597724605
H	0.2929539995	3.1276839654	-0.9906524149
H	-2.4430904126	2.5298833507	2.3380854326
H	-2.933486066	3.5505249575	0.9779150323
H	-1.6434308456	4.0885648096	2.0654860646
O	-2.7354291159	0.1268482139	1.787615931
O	-0.7403849016	-0.9889058761	2.7842496259
C	-1.9640851894	-0.4452753069	-1.4718232079
H	-1.1621235107	1.4307298312	-2.1302166017
C	-3.022782502	-0.5115157263	-2.3558750993
C	-1.9209946008	-1.3107729729	-0.3132765716
C	-3.0099394363	-2.2332965742	-0.100900282
C	-4.0680626187	-2.2656415281	-0.9741490694
C	-4.0588096637	-1.4211078936	-2.1072611175
H	-0.9521178867	-1.778959994	-0.1365577038
H	-2.9611276146	-2.9123152496	0.7439182839
H	-3.0852611661	0.1701963036	-3.1966465484
H	-4.8960989673	-2.9475602666	-0.8218659174
H	-4.9000715796	-1.4566283958	-2.7925159938
H	-2.4404717164	-0.403296033	2.57068827
H	-2.4404717164	-0.403296033	2.57068827

3.1.2 Lowest TS first run

TS 0008

$E(\text{RB3LYP}) = -1097.26674653 \text{ A.U.}$

First frequency = $-271.4263 \text{ cm}^{-1}$

C	-1.9555417974	0.0969958823	0.8724218198
C	-0.5590570266	0.425980407	1.4774423002
C	-2.293692451	-0.0802637328	-0.6209153265
C	-1.2873849681	-1.1587304731	-1.1107792922
C	0.0619057399	-0.5759487594	-1.587498353
N	0.564798074	0.2238274957	0.7586433887
C	0.6200519698	0.5459209479	-0.6888486695
H	-0.0888685685	-0.1638996889	-2.5862572079
H	0.8018027242	-1.3722586981	-1.6936366624
C	1.8219308398	-0.0044366132	1.4837282927
C	2.7733493958	1.1617671044	1.2747403392
H	2.2654603771	-0.927805417	1.0953473174
H	1.5739800191	-0.1490336651	2.5330242034
C	2.0068727579	1.0162506207	-1.1246007047
H	-0.021811212	1.4191367275	-0.8069453666
C	3.0097325004	1.3555500824	-0.2009652364
H	3.7188633834	0.9689121386	1.7900629055
H	2.3384167013	2.063390841	1.7240574629
C	2.2543857378	1.2021882677	-2.4928351435
C	3.4742316094	1.7002645248	-2.9421986705
C	4.4738904799	2.0238798807	-2.0240850622
C	4.2351951065	1.8475164418	-0.6648288532
H	5.0078885112	2.0909113035	0.0589703419
H	5.4301193924	2.4075042581	-2.3649086807
H	1.4878475173	0.9704581473	-3.2231294253
H	3.6405617635	1.8344954065	-4.0060547509
C	-2.4926852689	1.1691174074	-1.5172426761
H	-3.2859320566	-0.5445184637	-0.5995443416
H	-1.5410413357	1.6749258187	-1.6950920177
C	-3.4487682078	2.192788051	-0.8918646681
C	-3.0293999912	0.7107783588	-2.8833111954
H	-3.1840781383	1.5770480288	-3.532011392
H	-3.992008126	0.1995976712	-2.7711214879
H	-2.3428896951	0.031463829	-3.3959641978
H	-3.6254670221	3.0066653044	-1.6008069249
H	-3.0488200489	2.6239090823	0.0274820979
H	-4.415092445	1.7356079468	-0.6546482958
O	-2.9034144353	0.679267958	1.6091087573

O	-0.5929910309	0.6929268884	2.6821650477
C	-1.1041526937	-2.074393561	0.0806124296
H	-1.7160267535	-1.7219443992	-1.9459738001
C	-0.0550616655	-2.9594539344	0.2681692131
C	-1.9693590981	-1.7516922191	1.1900078657
C	-1.6538858584	-2.2584559434	2.4975349704
C	-0.5645483656	-3.0770692555	2.6726943746
C	0.2014115175	-3.4576630386	1.5488573161
H	-3.0388533387	-1.7490364154	0.9873251237
H	-2.3077684013	-2.0101954119	3.3263883947
H	0.6099403779	-3.2166220762	-0.547594005
H	-0.3081491359	-3.4623643195	3.6523053461
H	1.0443231762	-4.1266026839	1.6906310768
H	-2.4556204483	0.930863907	2.4527247926
H	-2.4556204483	0.930863907	2.4527247926

3.1.3 Additional TS first run

TS 0001

E(RB3LYP) = -1097.26550793 A.U.

First frequency = -363.3322 cm^{-1}

C	-1.435464588	0.0160608916	0.9109324442
C	-0.6699773824	1.3530961837	0.9999420256
C	-2.2421371852	-0.311499115	-0.3447898075
C	-1.2105647392	-0.8406678677	-1.3780318821
C	-0.4115181872	0.2885293283	-2.0465522209
N	-0.0084237144	1.8896923174	-0.0494309813
C	0.5347105004	1.2071317745	-1.2563398711
H	-1.1418881257	0.9372683837	-2.5332217844
H	0.1787275773	-0.1320834452	-2.8623818244
C	0.8327531552	3.0608391451	0.2755410293
C	2.1772864576	2.5587227504	0.8079401943
H	0.3180559557	3.6757752284	1.0099973643
H	0.9521782073	3.6374169419	-0.6433606313
C	1.9334218683	0.6718432807	-0.9152534735
H	0.6932507075	2.0365446664	-1.9522107144
C	2.7061090868	1.3557486056	0.0458729234

H	2.0570451615	2.2845916066	1.8624077729
H	2.9108811582	3.3707225683	0.7809870583
C	2.4765286678	-0.4440425612	-1.5644915294
C	3.7587142934	-0.8954381563	-1.264385165
C	4.522229087	-0.2259489828	-0.307281401
C	3.9933542117	0.8883720467	0.3370937445
H	4.5845004028	1.4136573981	1.0819669619
H	5.5222564849	-0.5702886123	-0.0646765209
H	1.8944354648	-0.9844220659	-2.3011617999
H	4.15562425	-1.7677164606	-1.7729877183
C	-3.1607664669	0.8480055034	-0.7974894551
H	-2.8829267245	-1.1538628409	-0.0609925309
H	-2.5341698665	1.6994996566	-1.0837235211
C	-4.0988684409	1.3181634107	0.3240965113
C	-3.9746358196	0.408856083	-2.0235950476
H	-4.6386343911	1.2179587885	-2.3393880183
H	-4.594610749	-0.4621791594	-1.785243575
H	-3.3410447073	0.1489634562	-2.875914231
H	-3.5556134526	1.752861008	1.1659019824
H	-4.7037858538	0.4889873953	0.7052364582
H	-4.7777251467	2.0828730534	-0.0634353849
O	-2.0839978681	-0.195776454	2.0490112255
O	-0.7456991957	1.9025827379	2.1082501212
C	-0.472924485	-1.8220117291	-0.5044544736
H	-1.7305433864	-1.3771085308	-2.174030069
C	-0.6307070469	-3.1923216239	-0.6010840609
C	0.0466608985	-1.2472611967	0.7077945616
C	0.3640964945	-2.1075630735	1.8074270483
C	0.1773997182	-3.4682433777	1.7016067833
C	-0.293971519	-4.0065390742	0.4890059363
H	0.7770691879	-0.4473297066	0.5956732387
H	0.7945826286	-1.6743180877	2.7039276859
H	-1.0697946741	-3.6317173429	-1.4900863361
H	0.4160252742	-4.1276626208	2.5276250271
H	-0.4349597048	-5.0795918077	0.4072143681
H	-1.7378024275	0.4955418458	2.6719864007
H	-1.7378024275	0.4955418458	2.6719864007

TS 0007

E(RB3LYP) = -1097.26568447 A.U.

First frequency = -344.4282 cm^{-1}

C	-1.9505333152	0.0939242525	0.9239796564
C	-0.8035092787	1.0969598218	1.1625135162
C	-2.5415479454	-0.2201420234	-0.4336225083
C	-1.3874345192	-0.8567961736	-1.2430791797
C	-0.4986347181	0.2038239592	-1.9274605025
N	0.0696820451	1.5435584493	0.2398003305
C	0.490478395	1.0662228259	-1.1055453022
H	-1.1544543865	0.878013424	-2.4756320311
H	0.0894685903	-0.2987782584	-2.6929149163
C	1.1058832595	2.4432341253	0.7984280623
C	2.2448352503	1.5552897184	1.2797819483
H	0.6708922016	3.0363174676	1.5974674481
H	1.4334426198	3.1068018878	-0.0048116173
C	1.9264653353	0.5010502571	-1.0119737508
H	0.5718443539	1.9930245837	-1.6850853478
C	2.7132171723	0.6772063694	0.140887833
H	1.8985586925	0.9571961482	2.1311404629
H	3.0768834826	2.1687204356	1.6396347097
C	2.4961886852	-0.1462701871	-2.1173614645
C	3.7632061793	-0.7191166848	-2.0491255866
C	4.499493296	-0.6339891697	-0.8669611326
C	3.9787186145	0.0822498535	0.2064360074
H	4.5665059296	0.2066788915	1.1115444382
H	5.4821155092	-1.0886411229	-0.795605767
H	1.9497687011	-0.2232204366	-3.0506183813
H	4.1691618085	-1.2304328066	-2.9156801411
C	-3.2751164296	0.9804035805	-1.0905364039
H	-3.3044476384	-0.985808711	-0.2531628661
H	-2.5517622333	1.7853086606	-1.2630161574
C	-4.3924244341	1.5452216827	-0.2024988614
C	-3.864528528	0.5397508841	-2.4398467928
H	-4.58822575	-0.2693413188	-2.292425061
H	-3.1062284218	0.1862470088	-3.1429385849
H	-4.3886289849	1.3766834188	-2.9088968571

H	-4.0130027975	1.9826922662	0.7220594192
H	-5.1135194419	0.7657251903	0.0652415938
H	-4.9286117449	2.3261218793	-0.7491071506
O	-2.8082210031	0.1965565389	1.9264650317
O	-0.7941451668	1.5176897296	2.3342476513
C	-0.5878420272	-1.6846316793	-0.2568694152
H	-1.7966386756	-1.4836243358	-2.0407816835
C	0.6805077738	-2.1904855457	-0.4863257371
C	-1.0971036353	-1.668637907	1.0840104275
C	-0.2335019868	-1.9806624536	2.1771783756
C	1.0686615188	-2.3629635257	1.9304048708
C	1.4990401141	-2.5227490559	0.5993325771
H	-2.1269276763	-1.9847999337	1.2276096797
H	-0.6314535004	-1.9600307305	3.1859869927
H	1.0829171584	-2.2453802357	-1.4886204531
H	1.7441359244	-2.591231284	2.7464790801
H	2.5121103817	-2.8576914995	0.4047659141
H	-2.3145207368	0.7389102554	2.6050352021
H	-2.3145207368	0.7389102554	2.6050352021

TS 0010

E(RB3LYP) = -1097.26170450 A.U.

First frequency = -246.8834 cm^{-1}

C	-1.6823468519	-0.1616640072	0.9790520765
C	-0.6591649915	0.9283912406	1.396889198
C	-1.9813106239	-0.4552184983	-0.4980964779
C	-0.7956308491	-1.3577355621	-0.9606545851
C	0.598383198	-0.6804453094	-1.078141116
N	0.5006613135	1.1276576598	0.733693729
C	0.7329575913	0.8158258296	-0.7067772822
H	0.9079786561	-0.7524578504	-2.1214810633
H	1.3452795406	-1.2447983014	-0.5113101982
C	1.4989607434	1.9644690389	1.4349237053
C	2.8963747409	1.4174852217	1.1772172835
H	1.245389646	1.9449104175	2.4922101512
H	1.4237693566	3.0000008636	1.0852003676
C	2.1050015012	1.2798272461	-1.1791268615

H	0.0029063289	1.3807087812	-1.285920102
C	3.1753207633	1.4773897617	-0.2997455208
H	2.9624045143	0.3917533168	1.5620763994
H	3.6260949661	2.0154669986	1.7303967334
C	2.3009952958	1.4483481836	-2.5553361712
C	3.5562220322	1.7782729604	-3.0587814352
C	4.6307506714	1.9517205385	-2.1831160565
C	4.4328719182	1.8133939754	-0.8115168492
H	5.2557947289	1.9787402153	-0.1220646233
H	5.6116338176	2.2130414234	-2.5669045354
H	1.4646358783	1.3231046729	-3.237807114
H	3.6932260382	1.907138686	-4.1274011745
C	-2.4147893718	0.7841523749	-1.3211299454
H	-2.8524655972	-1.1198895818	-0.4744347378
H	-1.8064716275	1.648077386	-1.0301663447
C	-3.8762207765	1.1453587979	-1.0178592112
C	-2.2262813965	0.5409570997	-2.8243312149
H	-2.8079726271	-0.3274343962	-3.1516687684
H	-1.1807725908	0.3660230151	-3.0933749052
H	-2.5748094737	1.4089323916	-3.3901043893
H	-4.165328756	2.040068782	-1.576444488
H	-4.031960259	1.3365958425	0.0454643117
H	-4.5436788998	0.3295004127	-1.3169314653
O	-2.7900366652	-0.0123888848	1.7193199538
O	-0.9378802285	1.4786638337	2.4712720327
C	-0.8630123096	-2.3432655814	0.1702741336
H	-1.0454678534	-1.8401686006	-1.9056961398
C	-1.3790901839	-3.6217960001	0.0943173163
C	-0.7224275944	-1.6840878904	1.4505164708
C	-1.140924251	-2.388439842	2.638292723
C	-1.6781917626	-3.647476917	2.5414977575
C	-1.7744200756	-4.2654113891	1.2741466064
H	0.232939723	-1.1783148884	1.5942004647
H	-0.9989629977	-1.9136997365	3.6035069829
H	-1.5344883892	-4.0997746892	-0.8663687742
H	-2.0040881595	-4.1840893414	3.4244954165
H	-2.1990728062	-5.2624428011	1.2096681485
H	-2.5168573903	0.5918791558	2.4551531646

H -2.5168573903 0.5918791558 2.4551531646

TS 0013

E(RB3LYP) = -1097.25965555 A.U.

First frequency = -358.2914 cm^{-1}

C -1.5162010112 0.0084919077 0.8048467796
C -0.7576234719 1.3545772261 0.9389420601
C -2.2298526731 -0.4219592768 -0.4738413779
C -1.1116395135 -0.8345196588 -1.4674347762
C -0.3688916783 0.3574156034 -2.0839843562
N -0.0028129438 1.8900267371 -0.0418728689
C 0.5648462166 1.2454776935 -1.2530004944
H -1.1296289121 1.0061662798 -2.5228644809
H 0.2230984088 0.0029745049 -2.9296520284
C 0.8447207966 3.0314617091 0.3582175372
C 2.1554600953 2.479717905 0.9229754831
H 0.3128610275 3.6306027345 1.0931490398
H 1.0133257474 3.637655968 -0.5338508827
C 1.9454168524 0.6787168834 -0.8930435483
H 0.74750358 2.0938524117 -1.9206047441
C 2.6922463731 1.3019128067 0.1274536943
H 1.9851764955 2.1614796812 1.9582012054
H 2.9048051363 3.2766488242 0.9638853099
C 2.4925247721 -0.4156732882 -1.5738412189
C 3.7533084284 -0.9070151582 -1.2457094554
C 4.4906595806 -0.2992486277 -0.2287171283
C 3.9583452876 0.7953252632 0.4458211549
H 4.5296461678 1.2737529857 1.2363843457
H 5.4734574648 -0.6753943806 0.0360714046
H 1.93179179 -0.9057875415 -2.360639286
H 4.1541506762 -1.7620639471 -1.7799005511
C -3.3654218271 0.5157816534 -0.980566148
H -2.7209708909 -1.3576174848 -0.1895032246
H -3.4408621478 0.3096648896 -2.0568884834
C -3.1547210794 2.0276127276 -0.8080458277
C -4.6974275554 0.1078618985 -0.33230914
H -4.9290460292 -0.9442684044 -0.5243811663

H	-5.5172506654	0.7137896007	-0.7284884807
H	-4.6600812333	0.2535762129	0.7517408389
H	-3.1060285163	2.3062870754	0.2495811011
H	-4.0098314279	2.5548492115	-1.2395555003
H	-2.2543056545	2.4008845312	-1.2968844931
O	-2.2487147894	-0.1710535437	1.8995876951
O	-0.9003670682	1.8930685768	2.0473028614
C	-0.3576967959	-1.7817366852	-0.5677568546
H	-1.5627702026	-1.3899636282	-2.2932590507
C	-0.3927502403	-3.1553380659	-0.7158526203
C	-0.0014790902	-1.2084594336	0.7081274486
C	0.2585545529	-2.0840143528	1.8134963266
C	0.1882333373	-3.4500739994	1.6533637733
C	-0.1058056686	-3.9789388232	0.3821746166
H	0.721727607	-0.3941902693	0.6784164562
H	0.5596044617	-1.6507612032	2.761544264
H	-0.7055358898	-3.5973737921	-1.6555773116
H	0.3865638948	-4.1179746881	2.4831626198
H	-0.1505249394	-5.056115558	0.2565412516
H	-1.9436406121	0.5418610449	2.5231316151
H	-1.9436406121	0.5418610449	2.5231316151

TS 0019

E(RB3LYP) = -1097.25563500 A.U.

First frequency = -235.7391 cm^{-1}

C	-1.5822664955	-0.3290362357	1.0421669229
C	-0.4955886003	0.6805684065	1.4780067887
C	-2.0210389073	-0.3680964397	-0.4286122671
C	-0.9534242952	-1.2730525601	-1.1026780309
C	0.483897273	-0.7013134599	-1.2110895815
N	0.5363324934	1.0700152287	0.6997535769
C	0.8243479864	0.7213445084	-0.7407213027
H	0.7324606431	-0.6948601614	-2.272940582
H	1.1858473565	-1.3997116957	-0.7475137002
C	1.3274232414	2.1823033978	1.2967480429
C	1.8861541254	3.1017338555	0.2175966357
H	2.1444768801	1.7585792992	1.8894963811

H	0.6672287783	2.7215560588	1.9727074573
C	2.2921353594	1.0362579709	-1.0663863727
H	0.2315233847	1.41799807	-1.3429939603
C	2.7839495684	2.289093859	-0.665253606
H	2.4311900844	3.9195349387	0.6951455578
H	1.0587606134	3.5507133447	-0.3479225408
C	3.128923853	0.1891495426	-1.8014444459
C	4.4237995309	0.5884291783	-2.1394919995
C	4.9003116083	1.8372923396	-1.7470580655
C	4.0787931091	2.6816174561	-1.0006631348
H	4.443174099	3.6491378969	-0.6680940283
H	5.9063304985	2.147835378	-2.010154904
H	2.7975883429	-0.7879184372	-2.1270267376
H	5.0562232682	-0.0837572854	-2.7102095451
C	-2.3655995533	1.0096832321	-1.0403992661
H	-2.9505318609	-0.9488737124	-0.4323804583
H	-1.582986115	1.7306660839	-0.7859770649
C	-3.6827045391	1.5476403638	-0.46254937
C	-2.4499092894	0.9101215688	-2.5695234239
H	-3.1926569886	0.162964316	-2.8702426727
H	-1.4921875693	0.6363678042	-3.0217134294
H	-2.7535144403	1.8720502183	-2.990965163
H	-4.5127077973	0.8719313034	-0.6967793485
H	-3.909730025	2.5246257111	-0.8985619734
H	-3.6362880892	1.658502899	0.6225345312
O	-2.6101474447	-0.2427120145	1.9004262631
O	-0.6560994636	1.0965238935	2.6373681731
C	-1.0151771139	-2.4029820648	-0.1148074724
H	-1.2976712647	-1.5940017639	-2.0853181074
C	-1.669139111	-3.6045425315	-0.2998470352
C	-0.6895628671	-1.9398221546	1.2165195388
C	-1.053544673	-2.7678884613	2.3413580296
C	-1.721552191	-3.9494205828	2.1409483368
C	-2.0081539159	-4.3710347259	0.8226509214
H	0.3112336276	-1.5221117679	1.3299012065
H	-0.7695703634	-2.4488009243	3.3386186724
H	-1.9666574778	-3.9263759415	-1.2915501183
H	-2.0081159937	-4.5762795884	2.976824924

H	-2.5360647565	-5.3083334325	0.6767736892
H	-2.2372892753	0.2498919323	2.6762713929
H	-2.2372892753	0.2498919323	2.6762713929

3.1.4 Starting TS second run

TS Input 2

E(RB3LYP) = -1097.26674653 A.U.

First frequency = -271.4263 cm^{-1}

C	-1.9555417974	0.0969958823	0.8724218198
C	-0.5590570266	0.425980407	1.4774423002
C	-2.293692451	-0.0802637328	-0.6209153265
C	-1.2873849681	-1.1587304731	-1.1107792922
C	0.0619057399	-0.5759487594	-1.587498353
N	0.564798074	0.2238274957	0.7586433887
C	0.6200519698	0.5459209479	-0.6888486695
H	-0.0888685685	-0.1638996889	-2.5862572079
H	0.8018027242	-1.3722586981	-1.6936366624
C	1.8219308398	-0.0044366132	1.4837282927
C	2.7733493958	1.1617671044	1.2747403392
H	2.2654603771	-0.927805417	1.0953473174
H	1.5739800191	-0.1490336651	2.5330242034
C	2.0068727579	1.0162506207	-1.1246007047
H	-0.021811212	1.4191367275	-0.8069453666
C	3.0097325004	1.3555500824	-0.2009652364
H	3.7188633834	0.9689121386	1.7900629055
H	2.3384167013	2.063390841	1.7240574629
C	2.2543857378	1.2021882677	-2.4928351435
C	3.4742316094	1.7002645248	-2.9421986705
C	4.4738904799	2.0238798807	-2.0240850622
C	4.2351951065	1.8475164418	-0.6648288532
H	5.0078885112	2.0909113035	0.0589703419
H	5.4301193924	2.4075042581	-2.3649086807
H	1.4878475173	0.9704581473	-3.2231294253
H	3.6405617635	1.8344954065	-4.0060547509
C	-2.4926852689	1.1691174074	-1.5172426761
H	-3.2859320566	-0.5445184637	-0.5995443416

H	-1.5410413357	1.6749258187	-1.6950920177
C	-3.4487682078	2.192788051	-0.8918646681
C	-3.0293999912	0.7107783588	-2.8833111954
H	-3.1840781383	1.5770480288	-3.532011392
H	-3.992008126	0.1995976712	-2.7711214879
H	-2.3428896951	0.031463829	-3.3959641978
H	-3.6254670221	3.0066653044	-1.6008069249
H	-3.0488200489	2.6239090823	0.0274820979
H	-4.415092445	1.7356079468	-0.6546482958
O	-2.9034144353	0.679267958	1.6091087573
O	-0.5929910309	0.6929268884	2.6821650477
C	-1.1041526937	-2.074393561	0.0806124296
H	-1.7160267535	-1.7219443992	-1.9459738001
C	-0.0550616655	-2.9594539344	0.2681692131
C	-1.9693590981	-1.7516922191	1.1900078657
C	-1.6538858584	-2.2584559434	2.4975349704
C	-0.5645483656	-3.0770692555	2.6726943746
C	0.2014115175	-3.4576630386	1.5488573161
H	-3.0388533387	-1.7490364154	0.9873251237
H	-2.3077684013	-2.0101954119	3.3263883947
H	0.6099403779	-3.2166220762	-0.547594005
H	-0.3081491359	-3.4623643195	3.6523053461
H	1.0443231762	-4.1266026839	1.6906310768
H	-2.4556204483	0.930863907	2.4527247926
H	-2.4556204483	0.930863907	2.4527247926

3.1.5 Lowest TS second run

TS 0001

E(RB3LYP) = -1097.27087472 A.U.

First frequency = -267.8252 cm^{-1}

C	-2.0836006188	-0.3341077353	-0.6243661752
C	-0.9508078341	0.4185967592	-1.3790878952
C	-1.904877784	-1.3952618145	0.4755796422
C	-1.0416647026	-0.6820402693	1.5484634431
C	0.4777288988	-0.7982144357	1.2963163994
N	0.3004825255	0.5132866271	-0.8851276898

C	0.9457558691	-0.6218717629	-0.1672341915
H	0.8127448567	-1.7900930933	1.6101665706
H	1.0096778441	-0.0875382309	1.9319038205
C	1.1462825398	1.5649271012	-1.4845271504
C	2.2670745391	1.9329506422	-0.5196732892
H	0.4986824678	2.4155084141	-1.694635798
H	1.5640145352	1.2161306378	-2.4356706396
C	2.4591336059	-0.5236687686	-0.1713498524
H	0.6894154321	-1.5211855427	-0.7265184058
C	3.1085050902	0.7142199581	-0.2515481424
H	1.8327239916	2.3300321555	0.4067381335
H	2.8718637655	2.7307840963	-0.9586782572
C	3.2068381067	-1.6941663959	-0.0061140958
C	4.5947436926	-1.6350314606	0.1001353451
C	5.2441139127	-0.4004905246	0.0307976886
C	4.5019421915	0.7645184649	-0.1552516144
H	5.004047257	1.7243971427	-0.2358603695
H	6.325567763	-0.3482900445	0.1049209979
H	2.7008202146	-2.6546336999	0.0384298597
H	5.1668378966	-2.5482238188	0.2272260489
C	-1.4905876384	-2.8334960963	0.0746863861
H	-2.9141986582	-1.5128745638	0.8862517071
H	-0.4617966797	-2.8472001673	-0.2912317675
C	-2.3813538707	-3.4129393961	-1.0315439076
C	-1.5504193646	-3.7289556302	1.3230494403
H	-1.2732646836	-4.7533005417	1.0601623612
H	-2.565238036	-3.7514718094	1.7356275593
H	-0.8717602513	-3.3940490027	2.1121150911
H	-2.1022114085	-4.4542297605	-1.2162671544
H	-2.2854081902	-2.8634792863	-1.9694208011
H	-3.4360822066	-3.3931098656	-0.7378610469
O	-3.0925001816	-0.5532518293	-1.4697791577
O	-1.3511718454	1.0426547213	-2.3687368614
C	-1.4859205152	0.7643461739	1.4998871176
H	-1.2409175937	-1.1016813487	2.5395724026
C	-0.7783159154	1.8439331654	2.0015393023
C	-2.5875350272	0.99560279	0.5984104503
C	-2.8528035606	2.3309878278	0.1390584129

C	-2.089244875	3.378891503	0.5950522841
C	-1.0862542313	3.1338291735	1.5575527495
H	-3.4968887899	0.4269950834	0.7858643531
H	-3.6834419799	2.4965141742	-0.538303487
H	0.0547593523	1.6995019239	2.6793303305
H	-2.2714452853	4.3909876942	0.2540209624
H	-0.5048132658	3.969127108	1.9346914617
H	-2.9147857483	0.0441112977	-2.2378559266
H	-2.9147857483	0.0441112977	-2.2378559266

3.1.6 Additional TS second run

TS 0008

E(RB3LYP) = -1097.26568425 A.U.

First frequency = -344.4003 cm^{-1}

C	-2.0839161403	-0.2148949414	-0.5259322842
C	-0.9345126128	0.0305333902	-1.5246143416
C	-2.1440711695	-1.3812651861	0.4369093641
C	-0.9346573717	-1.1918646766	1.3823920487
C	0.3614318049	-1.7978218314	0.8025046559
N	0.3069745387	-0.4861923652	-1.4538702122
C	1.1087472648	-1.1119128754	-0.3673784306
H	0.1408320813	-2.8212496747	0.5040899974
H	1.0779236097	-1.8915885691	1.6162895377
C	1.2083800339	0.0019073613	-2.5236419836
C	1.8392576821	1.2895319685	-2.0123923406
H	0.6350836892	0.1492790402	-3.4341584778
H	1.9635593614	-0.7683364181	-2.6946452646
C	2.2285914197	-0.1344618835	0.0577737389
H	1.6138576857	-1.9412708302	-0.8757886644
C	2.5139029385	1.025915448	-0.6846681754
H	1.0627678484	2.0585171914	-1.9220483398
H	2.5741824024	1.662857979	-2.7325377959
C	3.0310726607	-0.4314349527	1.1683215892
C	4.0085459098	0.453697287	1.6146733956
C	4.2172935301	1.6551314132	0.9365470587
C	3.4862332446	1.9183451737	-0.2178617811

H	3.6805277835	2.822152027	-0.7884582507
H	4.9658089256	2.3604549668	1.282363917
H	2.8952129286	-1.3597326908	1.7117081635
H	4.60051267	0.2042656149	2.4890417269
C	-2.2755572631	-2.7627478826	-0.2596307698
H	-3.0640329905	-1.2391601461	1.0151037107
H	-1.3856320483	-2.9342596975	-0.8756561482
C	-3.4993608497	-2.8427563082	-1.1826208237
C	-2.3647449152	-3.8644246616	0.8083599463
H	-3.2458089556	-3.7102030453	1.4408511421
H	-1.4878310962	-3.9010472207	1.4595134949
H	-2.4637456558	-4.8417058424	0.3284998065
H	-4.4193725784	-2.6091251231	-0.6364766078
H	-3.5901356451	-3.8594990517	-1.5751482779
H	-3.4306337675	-2.1602469662	-2.0309089153
O	-3.2223702603	0.1204567364	-1.1112766897
O	-1.2964882262	0.7430022352	-2.4792986234
C	-0.7927322457	0.3027202695	1.5904931476
H	-1.1223004215	-1.7041492144	2.3305696918
C	0.3181547985	0.9295593843	2.1292335154
C	-1.7730482978	1.0946550282	0.9053577513
C	-1.5029491816	2.4658323094	0.6135865876
C	-0.3279333437	3.0385104975	1.054101443
C	0.5465430506	2.2838049476	1.8592287167
H	-2.8178842045	0.8833842633	1.1170238921
H	-2.2517974454	3.0510463553	0.0908662458
H	1.0608933469	0.366915221	2.6781546655
H	-0.0978371331	4.0739108308	0.8319513326
H	1.4534717327	2.7444163442	2.2356170154
H	-2.9307524316	0.6178841334	-1.9272861425
H	-2.9307524316	0.6178841334	-1.9272861425

TS 0011

E(RB3LYP) = -1097.26674646 A.U.

First frequency = -271.2808 cm^{-1}

C	-1.9890951077	-0.2875464293	-0.716252485
C	-0.8286720224	0.5767009435	-1.2915402576

C	-1.8711715524	-1.3977210606	0.346528143
C	-1.1461935805	-0.707222637	1.5353811571
C	0.3948512834	-0.7700739308	1.4420771648
N	0.3451504631	0.6745134747	-0.6333907271
C	0.9551037885	-0.5042492849	0.0303035182
H	0.7052052444	-1.7711563762	1.7446637902
H	0.8458634316	-0.0802944181	2.1587414868
C	1.1703381179	1.8690729155	-0.8576698643
C	2.4497983252	1.4994418133	-1.5892853593
H	1.4063017359	2.2975597588	0.1225735333
H	0.5692982095	2.5829308774	-1.4167474556
C	2.482017471	-0.4597568386	0.0000839162
H	0.6869299581	-1.3518237198	-0.6006802242
C	3.1914400278	0.4511183408	-0.8005343894
H	3.0734803792	2.3882548687	-1.7226136369
H	2.1954336039	1.1299059239	-2.5906459873
C	3.1969907914	-1.4227397877	0.7276651884
C	4.5871654215	-1.4767612834	0.6773785571
C	5.2906349791	-0.5625812282	-0.107720732
C	4.589378401	0.3926584347	-0.8367050791
H	5.1265515419	1.1129975769	-1.4472287482
H	6.3746398459	-0.5930654424	-0.1490361527
H	2.6709932197	-2.1513519572	1.3335265421
H	5.1164879484	-2.2313535819	1.2499880369
C	-1.3784802064	-2.8084462603	-0.067144138
H	-2.9105936502	-1.5650428643	0.6500640227
H	-0.3128669321	-2.7928320692	-0.3065913693
C	-2.1189431952	-3.3507885532	-1.2962539295
C	-1.5655135602	-3.7612386099	1.1251313264
H	-1.2301167539	-4.7659839282	0.8546544362
H	-2.6216990915	-3.8253932517	1.4095098321
H	-0.9964307526	-3.4476676622	2.0045507003
H	-1.7999188699	-4.3789736057	-1.4893264833
H	-1.9209398362	-2.7597726313	-2.1920908909
H	-3.2016096844	-3.3581276255	-1.1323822786
O	-2.8935406583	-0.5042624975	-1.6729537767
O	-1.1604377972	1.268775236	-2.2583526886
C	-1.6441372809	0.7219318307	1.5037686384

H	-1.4382159002	-1.1784627875	2.4793831582
C	-1.0368719644	1.8050331553	2.117946415
C	-2.673276335	0.948658469	0.5173820933
C	-2.9633783931	2.2934710797	0.1010971194
C	-2.2955882489	3.3489816896	0.6732947013
C	-1.3687143729	3.1000744248	1.7093949755
H	-3.5664700461	0.3315189188	0.5964346865
H	-3.7366879269	2.4555927723	-0.641800903
H	-0.2604519843	1.661975296	2.8599246627
H	-2.4967038491	4.3684610751	0.3666318353
H	-0.8649517678	3.9407741156	2.175791586
H	-2.6832971784	0.15283883	-2.3797032782
H	-2.6832971784	0.15283883	-2.3797032782

3.2 Minor diastereoisomer

3.2.1 Starting TS

TS Input

E(RB3LYP) = -1097.25381744 A.U.

First frequency = -264.4836 cm^{-1}

C	-1.4661628778	-0.4432234621	0.8328755163
C	-0.3902180866	-1.5405317877	0.6872752465
C	-1.0326392423	1.0214838022	0.6795574406
C	-1.0869016513	1.270218175	-0.8554860936
C	-0.0653463068	0.5181375708	-1.7578151515
N	0.6245001723	-1.4849703496	-0.1911841163
C	0.9949551461	-0.4738048289	-1.2366292166
H	0.5045321471	1.2600414031	-2.3181812054
H	-0.6380192165	-0.0119956606	-2.5219240176
C	1.6115062071	-2.5874885496	-0.0241960844
C	2.9471778386	-2.2858650901	-0.71287218
H	1.1750735411	-3.5168166228	-0.402205524
H	1.764238318	-2.7112991324	1.0486055616
C	2.3513448162	0.1118608491	-0.8599779988
H	1.1871190827	-1.100140819	-2.1163120844
C	3.3405431743	-0.8413000183	-0.5640947164

H	2.8772283212	-2.5297287132	-1.7810571067
H	3.7058590386	-2.9507804968	-0.2936362746
C	2.6715742627	1.4691341434	-0.8394679711
C	3.9569345967	1.8816568404	-0.4830722276
C	4.9286763571	0.9368320103	-0.1542515543
C	4.6202884815	-0.4238997979	-0.2001173875
H	5.3777932386	-1.1650482326	0.0371375333
H	5.926169921	1.2572170164	0.1287284323
H	1.9284005429	2.217473871	-1.0872749448
H	4.1932298093	2.9403831366	-0.4594738281
C	0.2338165543	1.4097758948	1.4674192164
H	-1.8587885048	1.5992964875	1.1112151556
H	1.098614433	0.9105313135	1.0308586069
C	0.1505415664	0.9876047294	2.9425652588
C	0.4525451957	2.9258378473	1.3688486492
H	1.3815456884	3.2035925125	1.8738706253
H	-0.3702211324	3.4662483319	1.8498678424
H	0.5224312981	3.2742474202	0.335234072
H	0.123302894	-0.0973873043	3.0646490466
H	-0.7408351554	1.4024196297	3.424111166
H	1.0299382944	1.359618735	3.4759672396
O	-2.1705014967	-0.6783173244	1.9461934009
O	-0.5297482712	-2.4868984128	1.4809283356
C	-2.4669303866	0.7115273173	-1.077373191
H	-1.0558418235	2.3385263362	-1.0686911357
C	-3.6240691253	1.4487774576	-1.2309430474
C	-2.5300497851	-0.6797448502	-0.6886500696
C	-3.8241540425	-1.2797439596	-0.4846285
C	-4.9640354023	-0.5268823871	-0.6209888099
C	-4.859905969	0.8265667749	-1.0119526602
H	-1.84340718	-1.3497178664	-1.2044264994
H	-3.8797010535	-2.3360973009	-0.2445233967
H	-3.5788001592	2.5065496492	-1.4646918132
H	-5.9424004994	-0.9639696804	-0.4611019728
H	-5.7677540849	1.4119069084	-1.1196868816
H	-1.9223294841	-1.604065516	2.2027863152
H	-1.9223294841	-1.604065516	2.2027863152

3.2.2 Lowest TS

TS 0001

E(RB3LYP) = -1097.26850154 A.U.

First frequency = -359.8195 cm^{-1}

C	-2.1599452051	0.3500156509	0.4833362024
C	-0.9782708916	0.6818519429	1.4317297095
C	-2.0910468322	0.7031564172	-0.997368829
C	-1.1346625507	-0.3121773885	-1.6561453288
C	0.3610073615	0.0269961997	-1.4326499497
N	0.3046981437	0.7256524085	1.0219064718
C	0.8878275855	-0.1906935433	0.0022102061
H	0.5752539504	1.0473271012	-1.755235576
H	0.950606736	-0.6263510831	-2.0783843821
C	1.2249806778	1.4527500064	1.9234339118
C	2.3475262749	2.0822458624	1.1096343407
H	1.6322571114	0.7642721936	2.6725767969
H	0.6342742373	2.2043144626	2.4432336248
C	2.4067059583	-0.1263621324	-0.0330595273
H	0.6253522171	-1.2042044957	0.3148103011
C	3.116341944	0.9939347043	0.4118020668
H	3.0013883581	2.6469584472	1.779790865
H	1.9212511561	2.798501614	0.3958220063
C	3.0975935503	-1.2088787677	-0.5905543861
C	4.4820600626	-1.1678906245	-0.7320541432
C	5.1896637063	-0.0405958284	-0.3077750347
C	4.5072217158	1.0268667385	0.2710434382
H	5.0537152852	1.8944350537	0.6294344978
H	6.2691918644	-0.0025524888	-0.4117453722
H	2.5497090605	-2.0900733772	-0.9130207395
H	5.0067040856	-2.0135769402	-1.1643194967
C	-1.7656640277	2.2006061208	-1.2534856498
H	-3.1019589578	0.5277231444	-1.3833938487
H	-0.7613580133	2.4093398626	-0.8707529968
C	-2.7413822705	3.1441636161	-0.5377776339
C	-1.7781831711	2.4733942037	-2.7646336495
H	-1.5714467861	3.5301264467	-2.9541277118
H	-2.7601063682	2.2410971417	-3.1910827016

H	-1.0289005715	1.886939062	-3.3025901165
H	-3.7776527118	2.92752112	-0.8175584229
H	-2.523694651	4.1770029471	-0.8236927284
H	-2.6661979055	3.0775474686	0.54928486
O	-3.2834065356	0.6865881436	1.1035341855
O	-1.3484305526	1.0818773155	2.5465237316
C	-1.4069102534	-1.644994265	-1.0002133067
H	-1.3032052184	-0.3558325835	-2.7353255754
C	-0.652176374	-2.7949522865	-1.1935461493
C	-2.3249908905	-1.5888421975	0.0995067778
C	-2.3121011197	-2.6194139998	1.0896314142
C	-1.4830088064	-3.709784255	0.9272408049
C	-0.7032702954	-3.8186055976	-0.2418899932
H	-3.327694197	-1.2376773034	-0.1337873385
H	-3.0089556655	-2.5634984608	1.9190820393
H	0.0309655496	-2.8736875489	-2.0322469378
H	-1.4635984371	-4.5055147128	1.6626548508
H	-0.0870267427	-4.700260433	-0.3851718086
H	-2.9977348397	0.8877778579	2.0377586594
H	-2.9977348397	0.8877778579	2.0377586594

3.2.3 Additional TS

TS 0004

E(RB3LYP) = -1097.26548745 A.U.

First frequency = -283.7786 cm^{-1}

C	-1.9850789449	0.4627044723	0.3061647976
C	-0.7982743543	0.2850346961	1.2807910484
C	-1.8009296368	0.6573317293	-1.1878110872
C	-1.162062694	-0.6699508409	-1.6764833192
C	0.3698119895	-0.6248723829	-1.6403262739
N	0.3628208072	-0.3273770448	0.9871437365
C	1.0975323866	-0.6526601149	-0.2709278285
H	0.6825762228	0.255257249	-2.1955353315
H	0.752296073	-1.4784765842	-2.2044569529
C	1.2685475608	-0.5075971135	2.1441511584
C	2.2437722506	0.6580695814	2.1710552846

H	1.7951287689	-1.4544538911	1.9974212748
H	0.6723109621	-0.5690772345	3.0502454814
C	2.3981759089	0.1732955727	-0.3208317802
H	1.3859791897	-1.6966424833	-0.1074603316
C	2.9221071455	0.7970074305	0.8267052302
H	2.9924728011	0.5023908864	2.954173167
H	1.6987292262	1.5739096888	2.4295113008
C	3.1149510982	0.2624152077	-1.523784639
C	4.3001456541	0.988873918	-1.6070099907
C	4.794880824	1.6412836074	-0.478107309
C	4.1078636643	1.5339278953	0.7269306456
H	4.4973811227	2.018063112	1.6181771648
H	5.7146536349	2.2146663867	-0.5325042509
H	2.7579505334	-0.244025685	-2.4125761542
H	4.8315423698	1.0429188906	-2.5515523767
C	-1.059455993	1.9651740998	-1.5676145418
H	-2.811730496	0.7377011636	-1.6021642922
H	-0.0280172557	1.90670952	-1.2006555959
C	-1.6962281233	3.2166226396	-0.9470877753
C	-1.0363297142	2.1078583728	-3.0981061114
H	-2.0572333098	2.1956917203	-3.4852224337
H	-0.5617105073	1.2608977402	-3.6000741609
H	-0.4903424655	3.0115321644	-3.3815462963
H	-1.1902881832	4.1063704974	-1.3324934028
H	-1.6172541632	3.231371803	0.1410034291
H	-2.7566994044	3.2910662557	-1.2087070699
O	-2.8997738466	1.2317417077	0.8850702598
O	-1.0688115251	0.6820745353	2.4281657575
C	-1.6930437819	-1.7449499806	-0.7517889006
H	-1.4544469954	-0.8648755888	-2.7130572444
C	-1.0653658451	-2.9542747929	-0.5009655721
C	-2.7204962855	-1.2858449563	0.1416602725
C	-3.0037408097	-2.0245712587	1.3347126213
C	-2.3067217077	-3.1807144638	1.6067469416
C	-1.3745723778	-3.6617664245	0.6657978328
H	-3.5889170102	-0.8074898973	-0.305978995
H	-3.7879879166	-1.67393388	1.996728681
H	-0.2822653156	-3.3195198871	-1.1555833066

H	-2.494441099	-3.7425002742	2.5140699599
H	-0.8470374297	-4.5873458131	0.8724981894
H	-2.600676128	1.2850764698	1.8344601261
H	-2.600676128	1.2850764698	1.8344601261

TS 0007

E(RB3LYP) = -1097.26343415 A.U.

First frequency = -357.3603 cm⁻¹

C	-2.1726737447	0.377972946	0.2956276434
C	-1.0299335895	0.6894661375	1.3033145047
C	-2.0792854584	0.6187820005	-1.2045109457
C	-1.0579170681	-0.3875623239	-1.7494494287
C	0.4147319055	0.0031121971	-1.4655349612
N	0.2815821459	0.6683296788	0.9957732629
C	0.9081253112	-0.2192846772	-0.0193162565
H	0.5918078702	1.0372307961	-1.7679102896
H	1.0498483831	-0.6154094742	-2.101963042
C	1.1664528643	1.3219599452	1.9858299498
C	2.3309306163	1.9952974225	1.2726197694
H	1.5331173557	0.5760229637	2.7001635366
H	0.5602283581	2.0414274196	2.5307973953
C	2.4281580311	-0.1329805436	-0.0137191846
H	0.6585191219	-1.2420766427	0.2732905344
C	3.1196482566	0.9567007629	0.5246833803
H	2.9606172773	2.4950574861	2.0140168197
H	1.94938783	2.774152107	0.6008547257
C	3.1434883703	-1.175433402	-0.6168085618
C	4.5307896572	-1.1209718016	-0.7148939705
C	5.2198152249	-0.0200638044	-0.2001072074
C	4.5141501033	1.0042075733	0.42577547
H	5.0444357866	1.8487408831	0.8562837664
H	6.3016493406	0.0288528356	-0.269784072
H	2.6126370442	-2.0385756987	-1.0085770132
H	5.0718384307	-1.936274121	-1.183766984
C	-1.9342771272	2.1113990274	-1.6462494708
H	-3.0552023708	0.3003989153	-1.5849622445
H	-1.4116471484	2.0798593163	-2.6104892536

C	-1.139903071	3.0337388396	-0.710932016
C	-3.3303992877	2.7056081036	-1.8861261235
H	-3.91067266	2.7157026464	-0.9582582539
H	-3.8876483171	2.1267409057	-2.6291307018
H	-3.2503744455	3.7346282657	-2.2479469087
H	-1.1150297698	4.0393299095	-1.1389594767
H	-0.109367097	2.7118927399	-0.5629528501
H	-1.6159556542	3.1122109304	0.2717862941
O	-3.309984576	0.7965572383	0.8429520194
O	-1.4569497984	1.0968063108	2.3961339566
C	-1.350724165	-1.685771185	-1.034985231
H	-1.1661160372	-0.4832912779	-2.8337543935
C	-0.6043380648	-2.850135111	-1.1500135527
C	-2.2926498243	-1.5571256637	0.046120135
C	-2.2951950567	-2.5293427283	1.0965475007
C	-1.4731364786	-3.6330275576	1.0091844238
C	-0.6802458893	-3.8172870895	-0.1415756321
H	-3.3028105239	-1.2644233732	-0.2358421742
H	-3.0051349063	-2.4221267319	1.9096932872
H	0.0925749499	-2.980002114	-1.971001818
H	-1.4710097602	-4.3849683384	1.7894753796
H	-0.0719541767	-4.712077222	-0.2245172242
H	-3.0613921481	1.008493346	1.7859842722
H	-3.0613921481	1.008493346	1.7859842722

TS 0011

E(RB3LYP) = -1097.26352565 A.U.

First frequency = -303.4854 cm^{-1}

C	-2.1282113272	0.4865943569	0.3313822332
C	-0.8918866606	0.556550865	1.2703480418
C	-2.057510974	0.6748856419	-1.1746799396
C	-1.2082047438	-0.5168760312	-1.674235275
C	0.3007481642	-0.2152298994	-1.5953594593
N	0.3691907595	0.1860814519	0.9910396462
C	1.0245436597	-0.3501166974	-0.2533272167
H	0.4583400196	0.7803638454	-2.0014872636
H	0.830219883	-0.8997127339	-2.2631500432

C	1.2260367159	0.1844510813	2.2164978115
C	2.5539605614	-0.532398786	1.9992705352
H	0.6524428285	-0.2846343823	3.017188915
H	1.404136082	1.2236621514	2.5064098016
C	2.4483073756	0.2030422728	-0.3450654125
H	1.1259955626	-1.421632539	-0.0512553688
C	3.2424163913	0.0522215903	0.8024657542
H	2.3790033118	-1.6079952316	1.863297982
H	3.1561037078	-0.4205720797	2.9039893055
C	3.0080191037	0.7750837368	-1.4906931361
C	4.3398174411	1.1969342686	-1.487114349
C	5.1212222324	1.0523757595	-0.3420877259
C	4.5677791003	0.4825685604	0.8051985065
H	5.1640451187	0.3710822169	1.7060259288
H	6.1546712656	1.3836824646	-0.3404295819
H	2.4325358001	0.8945382141	-2.399921131
H	4.7615928832	1.6399141559	-2.3834159875
C	-1.6105415812	2.0927185507	-1.6160130579
H	-3.0838620531	0.5487044541	-1.5379355488
H	-0.6069727941	2.2891935235	-1.221071552
C	-2.5379312202	3.193820068	-1.0829308171
C	-1.565321077	2.1599188149	-3.1511757644
H	-0.8658089086	1.444475455	-3.5907050587
H	-1.2630998743	3.1602353002	-3.4722135898
H	-2.55749208	1.9584616755	-3.5695911468
H	-2.2282261865	4.1582894934	-1.495350858
H	-2.5158098893	3.2694545799	0.0047368054
H	-3.5746205756	3.0145932405	-1.3869491707
O	-3.1376293557	1.0962213343	0.9409202925
O	-1.2054156258	0.9611901206	2.4070073749
C	-1.5639483485	-1.6792416037	-0.774370148
H	-1.4422656948	-0.7381065353	-2.7192477926
C	-0.818550969	-2.8402643552	-0.640106919
C	-2.5650924846	-1.3678196293	0.2091565085
C	-2.6801415312	-2.1770359598	1.383924609
C	-1.8664662936	-3.2783476356	1.5384052833
C	-0.9783458832	-3.631788506	0.5032744514
H	-3.5229601981	-1.0129431719	-0.1660037943

H	-3.4429492943	-1.9358179682	2.1162169325
H	-0.0646688617	-3.1017512284	-1.3746600625
H	-1.9342722137	-3.8993862908	2.4237768972
H	-0.365403267	-4.5203502983	0.6149385884
H	-2.7942194113	1.2371679721	1.8705762579
H	-2.7942194113	1.2371679721	1.8705762579

TS 0013

E(RB3LYP) = -1097.26352559 A.U.

First frequency = -303.4729 cm^{-1}

C	-2.1338024845	0.5460765467	0.3545324098
C	-0.8801409699	0.6678933287	1.2647621965
C	-2.0913537624	0.6492195582	-1.1607961247
C	-1.2511840806	-0.5694157239	-1.6082604992
C	0.2588878243	-0.2649330264	-1.5748054376
N	0.3756319124	0.2814607694	0.9831579357
C	1.0077641869	-0.3244340207	-0.2410929884
H	0.4085251772	0.7060316372	-2.039368628
H	0.7759579337	-0.9864074024	-2.2127053803
C	1.2553196374	0.3483391862	2.1904696762
C	2.579198937	-0.3805286077	1.9891562699
H	0.6970211433	-0.0744434133	3.0269571988
H	1.4384471007	1.4021219949	2.4179207689
C	2.429345637	0.2217234625	-0.3905088941
H	1.1134065692	-1.3829280285	0.0190968381
C	3.2448813508	0.1352536049	0.7486208229
H	2.4021307974	-1.4619600862	1.9173289005
H	3.1981481292	-0.2183000202	2.8746959786
C	2.9672818091	0.7279129242	-1.5768339854
C	4.2987575435	1.1483815424	-1.6219784893
C	5.1015378754	1.0680344477	-0.4854644745
C	4.5699041512	0.5641562672	0.7022718524
H	5.1829900299	0.5031894952	1.5966217621
H	6.1347142299	1.3981974685	-0.5218363409
H	2.3748194865	0.7963377059	-2.4804110852
H	4.7034979692	1.5398639626	-2.5495607306
C	-1.6531472264	2.0396265843	-1.689530958

H	-3.1242840133	0.5035643426	-1.4971173735
H	-0.6423828582	2.2572177351	-1.3251989161
C	-2.5706485745	3.1697122786	-1.2019312666
C	-1.6368105094	2.0202994438	-3.2266201036
H	-2.6366009878	1.7963301743	-3.6143261298
H	-0.9454397432	1.2807508421	-3.6382500288
H	-1.3410103906	3.0007451516	-3.609064973
H	-2.5281215532	3.3064105351	-0.120850417
H	-3.6128202579	2.9744886155	-1.4758671288
H	-2.2690004912	4.1092040403	-1.6737073003
O	-3.131845793	1.1897863717	0.9475392255
O	-1.1724731258	1.1360893707	2.3825090086
C	-1.5896192706	-1.6789988102	-0.6378446229
H	-1.5047390185	-0.8489671502	-2.6345856099
C	-0.8414270688	-2.8311293179	-0.4523290609
C	-2.5722824449	-1.3119563673	0.3451354742
C	-2.6649966254	-2.0535729505	1.565606826
C	-1.8481382479	-3.1449594824	1.7666816076
C	-0.9794568159	-3.5568115073	0.7366614278
H	-3.5371216051	-0.9780872113	-0.0314331782
H	-3.4140334266	-1.7709221733	2.2972940066
H	-0.1013610433	-3.1341551166	-1.1849650053
H	-1.8990895974	-3.7150355713	2.6867830127
H	-0.3641921586	-4.4380803184	0.8867430657
H	-2.7711648657	1.3825879196	1.8612037345
H	-2.7711648657	1.3825879196	1.8612037345

TS 0014

E(RB3LYP) = -1097.26236574 A.U.

First frequency = -287.0972 cm^{-1}

C	-2.1271148486	0.4664936956	0.1351888569
C	-0.9339827885	0.5294200654	1.1263636305
C	-2.0088094602	0.5358406996	-1.3747495796
C	-1.150362689	-0.687306329	-1.7565734848
C	0.3535657165	-0.3803287369	-1.6672357847
N	0.3202888042	0.0970371558	0.9157507403
C	1.0409139173	-0.4268632026	-0.2981686218

H	0.5034321498	0.586712795	-2.141104969
H	0.9064616844	-1.098743305	-2.2782846321
C	1.1246917634	0.1077915736	2.1754857279
C	2.4981168113	-0.5316163818	1.9979498936
H	0.5438598544	-0.4073943851	2.9429861245
H	1.2370965299	1.1477571943	2.4927255957
C	2.4325383307	0.2042634262	-0.3491351787
H	1.191059242	-1.4858249971	-0.0636904641
C	3.1917377268	0.1006383701	0.8276743462
H	2.3920185983	-1.6143422414	1.8492488382
H	3.0627526909	-0.3925443201	2.9227626399
C	2.9956854102	0.8121752788	-1.4740895035
C	4.2972757503	1.3173834213	-1.421788481
C	5.0434447233	1.2197713623	-0.248746564
C	4.4862943704	0.6132205402	0.8781153992
H	5.0563345497	0.5371207096	1.7993605861
H	6.0530905635	1.6157789216	-0.2093738618
H	2.4468436821	0.8952918108	-2.4037147103
H	4.7230032913	1.7879275367	-2.3019893015
C	-1.6052274136	1.9378179164	-1.9264435317
H	-3.019961121	0.347274289	-1.7468190915
H	-1.1019364075	1.7533813307	-2.883682509
C	-0.6577276818	2.7564078705	-1.0334639013
C	-2.8694824882	2.7584917909	-2.2211012677
H	-2.6022092069	3.7280570441	-2.6509713926
H	-3.4377407171	2.9386161844	-1.303757071
H	-3.5226218469	2.2408243742	-2.9303834946
H	-1.1348149685	3.0079717653	-0.0809093434
H	-0.418679118	3.6990334493	-1.5328666552
H	0.2875974646	2.2565894047	-0.815136782
O	-3.1265611189	1.1774373205	0.6478616452
O	-1.2841423296	0.9714241872	2.2373628762
C	-1.5510254778	-1.7715648392	-0.7779280256
H	-1.3622763627	-0.9793732906	-2.789929931
C	-0.8145375399	-2.9140566142	-0.5106656931
C	-2.5910699851	-1.3723982831	0.1378464052
C	-2.7509028004	-2.0776026198	1.3741211769
C	-1.9423868362	-3.155903467	1.6593647639

C	-1.0162486525	-3.5981296881	0.6944128452
H	-3.5360166149	-1.056073613	-0.3001596147
H	-3.5411259823	-1.7753322937	2.0527263294
H	-0.0340505318	-3.2412695381	-1.1887114518
H	-2.0430123063	-3.6940260735	2.5944086593
H	-0.4073804845	-4.4705172103	0.9091115826
H	-2.8354547282	1.3457569786	1.5885580785
H	-2.8354547282	1.3457569786	1.5885580785

4 Black rearrangement

4.1 Major enantiomer

4.1.1 Starting TS

TS input

E(RB3LYP) = -1488.75209795 A.U.

First frequency = -224.4010 cm^{-1}

O	-1.8460327865	-1.8637924436	1.2323555539
O	0.2774701639	-1.4349212642	1.9609074965
O	0.3466138726	0.5645705621	-0.466668626
O	0.4361536788	-0.6398372474	-2.4463551994
O	-0.7715474054	3.1621389299	1.5155974617
O	-1.4253860328	0.9941380412	1.6752409704
N	-1.5894396263	-0.3072023996	-1.3619912452
N	-3.6723452652	-0.1046898833	-0.792304184
C	-0.4655448215	-3.2570887352	-1.1795355945
C	-0.6448331144	-1.8926794669	0.9897053644
C	0.0807269933	-2.2528114941	-0.2064292402
C	1.5410897322	-1.6383639373	1.454257438
C	2.728592946	-1.3760710839	2.1143075867
C	1.4825023112	-2.1942825064	0.1631563454
C	2.671814216	-2.5342077056	-0.4838137171
C	3.888686348	-2.2892485682	0.1700445996
C	3.9177107722	-1.7078816746	1.4430257678
C	-0.1052274297	-0.3840494593	-1.3787781066
C	0.5478995199	1.6045404431	2.8099042445

C	-0.5996330688	2.0411297556	1.9484623042
C	-2.4314612567	1.1971702889	0.6982196334
C	-3.8414521118	0.9444632325	1.2825696889
C	-4.6990320006	0.4734368011	0.0891824301
C	-2.4211513269	0.2089906943	-0.4386715195
C	-2.3593740837	-0.9687380838	-2.3150141537
C	-3.6690526073	-0.836346191	-1.9605603065
H	-0.1252255491	-4.2710921756	-0.9369358705
H	-1.5579907321	-3.2571888626	-1.1628060263
H	-0.1278828025	-3.0271228544	-2.19645097
H	2.7353612279	-0.9473499753	3.110667163
H	2.652029481	-2.9731675257	-1.4764391681
H	4.8222384027	-2.5461254536	-0.3218508211
H	4.8705954521	-1.5181702109	1.9275057642
H	0.9566733352	2.4643913847	3.3399625219
H	0.2486549496	0.8130497579	3.496378841
H	1.3140296072	1.1890276576	2.1472541307
H	-1.8869573611	-1.4685758316	-3.1420232854
H	-4.5707506164	-1.1925722933	-2.430139684
H	-2.3356312423	2.2081425771	0.2891190614
H	-4.2487316178	1.8311960841	1.7679961985
H	-3.7436033106	0.1393350573	2.01411275
H	-5.1923489514	1.2990255362	-0.4300799559
H	-5.4398024615	-0.2824978905	0.3514276612
C	1.3726545869	1.4253938965	-0.877096423
C	2.6826372683	0.97227572	-1.0042859528
C	1.0428968078	2.7653891918	-1.0704059192
C	3.6812797808	1.8877959198	-1.3414895174
C	2.0518871765	3.6725038019	-1.3997300743
C	3.3716538418	3.2360212998	-1.5393863779
H	2.905713668	-0.0728252137	-0.8403555493
H	0.0163635885	3.0847218871	-0.9369833425
H	4.7059096363	1.542686792	-1.4437783057
H	1.8035432167	4.7193449784	-1.5463468363
H	4.154537001	3.9430381409	-1.7964060048
H	4.154537001	3.9430381409	-1.7964060048

4.1.2 Lowest TS

TS 6-311++G(d,p) 0011

E(RB3LYP) = -1489.12331988 A.U.

First frequency = -241.1707 cm⁻¹

O	-1.6329068304	2.5052251665	0.1981990834
O	0.3425970396	2.367841263	-0.9206360409
O	0.2726893734	-0.7317437746	0.0972387842
O	0.502272227	-0.7642503244	2.3947286585
O	-0.9608860576	-1.8201609261	-2.7800420635
O	-1.595719114	0.1426752042	-1.8480910737
N	-1.539510984	-0.2414727535	1.4403415373
N	-3.6401993411	0.0044845229	0.9766989187
C	0.1125379654	2.1888460724	2.7608133839
C	-0.435954044	2.2685874223	0.2566739187
C	0.4055951908	1.8128344236	1.3362278887
C	1.6476509035	2.1079442561	-0.574517167
C	2.7350538016	2.1733292672	-1.425034754
C	1.7507994838	1.7926843345	0.7899681257
C	3.0097792132	1.5262435339	1.3269333169
C	4.1267429336	1.5766098216	0.484683771
C	3.9940824951	1.8949221502	-0.8705741184
C	-0.0662467973	-0.3684954838	1.3914932659
C	0.1965906075	0.209194446	-3.3745726557
C	-0.8276644259	-0.6239574639	-2.6672523287
C	-2.547392343	-0.5181532302	-1.0237470307
C	-3.9807163285	-0.0183707744	-1.332906516
C	-4.7441126587	-0.0674781497	0.0059913166
C	-2.4356158689	-0.1931629451	0.4389733507
C	-2.2206033757	-0.0530370111	2.6391277735
C	-3.542013983	0.0928164602	2.3479736066
H	-0.9595968704	2.3177655754	2.9178828704
H	0.4783129025	1.420067135	3.4477650944
H	0.6031804502	3.1325318714	3.0243333903
H	2.6176993995	2.4334446687	-2.4698383557
H	3.1190955369	1.2805711532	2.3767531825
H	5.1106466503	1.3652904684	0.8880989201
H	4.8723843984	1.9299863785	-1.5046777006

H	0.5171702533	-0.2996325707	-4.281601307
H	-0.1845082027	1.2055265322	-3.5917091243
H	1.0520622528	0.3199633838	-2.7046793475
H	-1.6908189436	-0.0422971954	3.5733246714
H	-4.393791455	0.2494468008	2.9858789019
H	-2.4484899808	-1.5979549988	-1.1553745939
H	-4.4595204585	-0.6158877546	-2.1059210446
H	-3.8982331911	1.012453168	-1.6793005463
H	-5.2801298886	-1.0063341728	0.152068407
H	-5.4278865492	0.7669078009	0.1501312712
C	1.1919916095	-1.775567687	-0.0572295918
C	0.8431893882	-3.0716625116	0.3099907011
C	2.4106271252	-1.4938628135	-0.6573606983
C	1.7432603237	-4.1075044886	0.0689222555
C	3.3013405784	-2.5391488345	-0.9032482516
C	2.9722279993	-3.844889561	-0.5402270785
H	-0.1177306591	-3.2603752654	0.7725449227
H	2.6550067192	-0.4731408601	-0.9151251518
H	1.4810891792	-5.1205621488	0.3518330545
H	4.2550115227	-2.3274619659	-1.3731483431
H	3.6676150858	-4.6543172588	-0.7299541712
H	3.6676150858	-4.6543172588	-0.7299541712

4.1.3 Additional TS

TS 6-31G(d,p) 0001

E(RB3LYP) = -1488.75700237 A.U.

First frequency = -87.4323 cm^{-1}

O	-2.0073840185	2.4087523304	1.7752658218
O	-0.2599237256	3.0283761677	0.4113069268
O	1.282189056	-0.8685611377	-0.9580786249
O	-0.244343323	-1.7258836498	0.5206438059
O	-3.0717082233	-1.9932092379	-1.3052551964
O	-3.0985301983	-1.5844371329	0.9159184319
N	-0.7669351931	0.0189916137	-0.8860530691
N	-2.5335957682	1.2317729203	-1.1413859988
C	0.0640952986	0.4827205532	3.1507528281

C	-0.7938114109	2.26168738	1.5122185221
C	0.2261153758	1.444871284	2.0156050533
C	1.0495620092	2.6608972413	0.2642696739
C	1.9234896122	3.1219536932	-0.703006609
C	1.4014845397	1.6920932997	1.2403499842
C	2.7169078056	1.1979761077	1.2343531477
C	3.6133192239	1.6548980091	0.2607495513
C	3.2308506521	2.6004329	-0.6999293054
C	0.1098500327	-0.9627016434	-0.3406368881
C	-3.3413273129	-3.838549187	0.2335389269
C	-3.1578100973	-2.4001386471	-0.1624584791
C	-2.9202457986	-0.1829777239	0.6963067051
C	-4.2360117393	0.5473721084	0.305279293
C	-3.819042425	1.7179556437	-0.6111186141
C	-2.0244676239	0.2361065052	-0.43611663
C	-0.5112797439	0.9114563222	-1.9367991991
C	-1.6216965695	1.6792856513	-2.0826024758
H	-0.9152573432	0.6196949033	3.6215706346
H	0.1267749263	-0.5660445218	2.8254371352
H	0.8275277462	0.6220458426	3.9286496053
H	1.60340086	3.856569371	-1.435889154
H	3.0309293227	0.4587562155	1.9651390526
H	4.6267600766	1.2616567271	0.2473692651
H	3.9437476868	2.9365989772	-1.4470073682
H	-4.3270700491	-4.1715446326	-0.1041711038
H	-2.5912417288	-4.4401601014	-0.2846389259
H	-3.2571317592	-3.9766389826	1.310642202
H	0.4373838291	0.9190276018	-2.4424874472
H	-1.8321644349	2.4956490637	-2.7524536187
H	-2.508449511	0.2112775492	1.625504055
H	-4.7705857557	0.8953704694	1.187806612
H	-4.8670167501	-0.1544107312	-0.2439737473
H	-3.6044806615	2.6203210388	-0.0363226001
H	-4.5143080999	1.9182956927	-1.4260969908
C	2.3550297691	-1.7289752443	-0.6533320411
C	3.1532858283	-2.0622466221	-1.7418466072
C	2.6443520797	-2.152098852	0.6410891571
C	4.2798505589	-2.8575815687	-1.5295966507

C	3.7739176834	-2.9499355602	0.8333452522
C	4.5904743978	-3.3043132468	-0.2431468033
H	2.8901521692	-1.6969724508	-2.7282985064
H	2.0148478025	-1.8651036215	1.4709204094
H	4.9113645006	-3.1247878707	-2.3706543793
H	4.0154397127	-3.2890064761	1.8356348833
H	5.4669391323	-3.9229307798	-0.0792205709
H	5.4669391323	-3.9229307798	-0.0792205709

TS 6-31G(d,p) 0003

E(RB3LYP) = -1488.75732104 A.U.

First frequency = -84.3080 cm⁻¹

O	-1.5495721255	2.3167380019	0.7598041644
O	0.5078483193	2.7770575393	-0.1703309631
O	0.9418494117	-0.7870334857	-1.2102869882
O	-0.4060521233	-1.6348360119	0.4430288172
O	-3.3479325274	-2.2648629571	-0.9370579601
O	-3.1949601063	-1.5043894961	1.1850120466
N	-1.1582984154	-0.0452458341	-1.0498937064
N	-3.0432426818	0.9797577457	-1.3283537293
C	0.0435204859	0.5647752302	2.8247414347
C	-0.3156905869	2.130732605	0.8228293341
C	0.5153110873	1.3800051459	1.6634808055
C	1.8053356816	2.4505330782	0.1124393298
C	2.9268060838	2.891793348	-0.5671298033
C	1.8655050454	1.5982128868	1.2450808337
C	3.1287320985	1.1973966921	1.7089479006
C	4.2737520183	1.6475204385	1.0412819451
C	4.1831714241	2.4757668482	-0.0862907477
C	-0.1730619229	-0.9018117867	-0.4856236681
C	-3.2762668855	-3.8511878608	0.8863153036
C	-3.2775299348	-2.4864345655	0.2561544948
C	-3.150577113	-0.149498792	0.7331648225
C	-4.5488012728	0.4210535717	0.3661701386
C	-4.2950650766	1.4719194009	-0.7355535474
C	-2.3883349686	0.1519752171	-0.5266307278
C	-1.0493837103	0.7306233657	-2.2153249859

C	-2.2306142392	1.3794848161	-2.3743504084
H	-0.0031315718	-0.508594999	2.5922566075
H	0.7037590248	0.6806156566	3.6938955761
H	-0.9620613992	0.8760654557	3.1295069197
H	2.8341724588	3.5436359754	-1.4305517146
H	3.215003959	0.5437222529	2.572578702
H	5.2532271506	1.337335084	1.3960959363
H	5.0855159347	2.8050436248	-0.5927777817
H	-4.263118082	-4.3028942149	0.7486464602
H	-2.5482563035	-4.4742693615	0.3624038493
H	-3.0399002075	-3.8066952346	1.948641397
H	-0.1498485185	0.7266943846	-2.804297654
H	-2.5581540155	2.0686136067	-3.1346538596
H	-2.6773412153	0.4105229062	1.5392738018
H	-5.0484844236	0.8488847164	1.2344335178
H	-5.1572004816	-0.3949299312	-0.0287688782
H	-4.0947663619	2.463095827	-0.3229047951
H	-5.0825088126	1.5263253931	-1.4871276377
C	2.0631571078	-1.5948423316	-0.9319052168
C	3.2847528192	-0.9355651611	-0.9281708308
C	1.9507060754	-2.9717980491	-0.7616689797
C	4.4439385072	-1.6870721757	-0.7335087476
C	3.1215782812	-3.7069774631	-0.5654236511
C	4.3653614327	-3.0698425546	-0.5507679112
H	3.3149540567	0.1396877754	-1.0543660155
H	0.9803990914	-3.4518646918	-0.7739153446
H	5.4049740517	-1.1831679571	-0.7159547092
H	3.056702371	-4.7814581018	-0.4262846187
H	5.2694916034	-3.6503305264	-0.3964813121
H	5.2694916034	-3.6503305264	-0.3964813121

TS 6-31G(d,p) 0008

E(RB3LYP) = -1488.75158089 A.U.

First frequency = -210.8010 cm^{-1}

O	-1.6700236567	2.4385306392	0.1524975726
O	0.1522669237	1.9639791347	-1.144316471
O	0.3115638783	-0.8679877281	0.4451341313

O	0.566010133	-0.4005337192	2.7147002283
O	-0.806257281	-1.3148006148	-2.8620513248
O	-2.1834565505	0.0440309433	-1.6760750811
N	-1.4677984177	-0.1257449455	1.6412172313
N	-3.5800981972	-0.1356908337	1.1536953097
C	0.3483518288	2.5280334709	2.5144481922
C	-0.4755165929	2.1693882558	0.1165636931
C	0.4927092463	1.9193395655	1.1515034043
C	1.4874178964	1.7267641284	-0.9081315909
C	2.4530549819	1.5278595333	-1.8768616349
C	1.7591266864	1.7255866181	0.4725966576
C	3.070553235	1.502824429	0.8991742009
C	4.0664860458	1.2910041832	-0.0628296399
C	3.7646746535	1.2999436619	-1.4297826305
C	0.0042249394	-0.2531716401	1.6376432663
C	-1.3542995833	0.8904474527	-3.7065841486
C	-1.3837101813	-0.2548144679	-2.7344163485
C	-2.4206213655	-0.9900907357	-0.7038192773
C	-3.9112495741	-1.41311106	-0.7630231796
C	-4.6549988431	-0.4618348365	0.2026815801
C	-2.3595456684	-0.4004443517	0.6741917599
C	-2.1599729602	0.3447114764	2.7474607598
C	-3.4907651997	0.3444756735	2.4390172344
H	-0.7029481124	2.7446984548	2.7234154373
H	0.7276679105	1.8500954277	3.2872883441
H	0.9051429566	3.4703679386	2.5928481518
H	2.2005866637	1.5393669329	-2.9320831109
H	3.3091382502	1.4877183118	1.9582823149
H	5.0891799744	1.1121226859	0.2565968838
H	4.5523026493	1.1299226008	-2.1575788681
H	-0.6662357342	0.6588067437	-4.5188697785
H	-2.3597562443	1.0539104673	-4.1056095429
H	-1.0413355861	1.7942516571	-3.1823203605
H	-1.6346999222	0.6100606644	3.6479975798
H	-4.3522322724	0.6214325891	3.0232722904
H	-1.719259091	-1.8073548808	-0.857231823
H	-4.0032535287	-2.442085046	-0.4061887628
H	-4.2892085018	-1.3587155164	-1.7839337784

H	-5.488418256	-0.9325970698	0.7235565907
H	-4.9959315008	0.4574540339	-0.2789845825
C	1.464490958	-1.6342251557	0.2682394149
C	2.0921338409	-2.3586171566	1.2858105147
C	1.9097509442	-1.7118715222	-1.051633553
C	3.2013351682	-3.1436904387	0.9618262117
C	3.0118693092	-2.5079973774	-1.3564308615
C	3.668473729	-3.2225540472	-0.3514224435
H	1.7317406393	-2.2993840423	2.3018902184
H	1.3849759665	-1.1545678909	-1.8152229767
H	3.697550033	-3.7019169469	1.7503995702
H	3.3588804493	-2.5636044817	-2.3839166354
H	4.5313941077	-3.8368375297	-0.5894400219
H	4.5313941077	-3.8368375297	-0.5894400219

TS 6-31G(d,p) 0009

E(RB3LYP) = -1488.75686172 A.U.

First frequency = -79.6070 cm^{-1}

O	-1.6299877977	2.0275152365	1.0452754545
O	0.3614645947	2.694204933	0.1040854031
O	1.0775115915	-0.5996662842	-1.1907230782
O	-0.4579135003	-1.686368361	0.1429396648
O	-3.0976512039	-2.3677106194	2.0863957498
O	-3.5465999775	-1.6031541035	-0.005812634
N	-1.0398312634	0.1022577917	-1.1833979684
N	-2.9141456988	1.1493936218	-1.4840955097
C	0.0989494567	0.0762107639	2.7718661229
C	-0.3876045175	1.8922048849	1.03481671
C	0.5030005837	1.0532749172	1.7157960338
C	1.6770938837	2.3465961668	0.246312091
C	2.7410162423	2.8707395822	-0.4664650694
C	1.8214867894	1.3469531321	1.2403065876
C	3.1111968964	0.8724600147	1.5247089536
C	4.1976472771	1.3929195672	0.8147582978
C	4.0226164905	2.3746095464	-0.1709291875
C	-0.1060371613	-0.8201569158	-0.6234351184
C	-3.7963266835	-3.925259269	0.3789204803

C	-3.4313365008	-2.5759927747	0.9403862427
C	-3.1454067142	-0.270356629	0.3814735415
C	-4.3333507442	0.725383966	0.3435615688
C	-4.2837542513	1.4427725535	-1.0334603401
C	-2.2882042447	0.280275059	-0.7013413007
C	-0.8725442198	0.961796083	-2.2792419341
C	-2.0541205042	1.6109499594	-2.4637803392
H	0.0852206942	-0.9578961433	2.3998288548
H	0.7772158258	0.1043513911	3.6340220997
H	-0.9112207274	0.3019605983	3.129688128
H	2.5835563245	3.6339751351	-1.2224774032
H	3.2593341469	0.0957397187	2.2692237632
H	5.1967399096	1.0188479525	1.0217873175
H	4.8823379733	2.7585161731	-0.712213749
H	-3.9582949933	-3.8902143741	-0.6978712779
H	-2.9946572462	-4.6286096969	0.6161484951
H	-4.7047008198	-4.2781639946	0.8757036521
H	0.0640499165	1.0184540858	-2.8046142055
H	-2.3436103154	2.3459561	-3.196122988
H	-2.6396734549	-0.298743635	1.3417401184
H	-4.1822383422	1.4548751965	1.138439322
H	-5.2768434489	0.2028281909	0.5017967728
H	-4.4182849367	2.5216020807	-0.9523984729
H	-4.9927378623	1.043188104	-1.7616859032
C	2.2484211078	-1.3229196637	-0.9132584498
C	3.305542453	-0.9863647881	-1.755409601
C	2.3878800877	-2.2615255412	0.107711225
C	4.5407719434	-1.6032248622	-1.5728258951
C	3.6352060682	-2.8689450474	0.2733496386
C	4.7101191759	-2.5470946094	-0.5567164865
H	3.152484283	-0.2354367379	-2.5220248702
H	1.561269782	-2.5035039611	0.757656022
H	5.3700502823	-1.3401402316	-2.221672389
H	3.7603014685	-3.5987714214	1.0672054568
H	5.6730667307	-3.0263653622	-0.4120080118
H	5.6730667307	-3.0263653622	-0.4120080118

TS 6-31G(d,p) 0011

E(RB3LYP) = -1488.75261371 A.U.

First frequency = -216.9824 cm^{-1}

O	-1.7002291837	2.3973374973	0.1254792028
O	0.2957290778	2.3034862899	-0.9839860156
O	0.2847837088	-0.7504724149	0.0717743627
O	0.5492163213	-0.7714633733	2.3705622927
O	-0.9376617031	-1.8911669124	-2.6334764187
O	-1.5999511295	0.1371294534	-1.8513012157
N	-1.5161089382	-0.2941883429	1.4401953457
N	-3.6210357056	0.0037823263	1.0159529679
C	0.0340894701	2.1887327001	2.7101163204
C	-0.4879189086	2.2165210587	0.1957538672
C	0.3623230852	1.8260711817	1.2910484066
C	1.6044132275	2.0902582089	-0.6219219685
C	2.6973063285	2.1548202501	-1.4699139673
C	1.7099676186	1.8260804333	0.7570267053
C	2.974367182	1.6047829901	1.3071084588
C	4.0955477614	1.65837331	0.4678358128
C	3.9620516937	1.9293486683	-0.8997417418
C	-0.0477405201	-0.4019158378	1.3700753102
C	0.2610650625	0.0954284849	-3.3011074357
C	-0.8032978467	-0.6866376755	-2.5894057776
C	-2.5734514686	-0.4728134138	-1.0203060674
C	-3.9704208679	0.1384516985	-1.2853984706
C	-4.7320111671	0.0284734088	0.0522261961
C	-2.4253732196	-0.1966756563	0.4525859032
C	-2.1773068695	-0.1308650633	2.6556223516
C	-3.5013058673	0.0502077693	2.3883191926
H	-1.0448090282	2.3097944352	2.8355584683
H	0.3838927633	1.4126973053	3.4006259284
H	0.5129142448	3.1320411652	3.0008378088
H	2.5767591395	2.3756494215	-2.5250598465
H	3.0826835345	1.3923953938	2.3661574719
H	5.0839025885	1.4851933242	0.8834397101
H	4.8439287556	1.9668575916	-1.5318503548
H	0.5151999032	-0.4040316537	-4.236402822
H	-0.0437077023	1.1277781096	-3.4667314967

H	1.1450950718	0.1066530793	-2.6566916132
H	-1.6286403808	-0.159136341	3.5802533253
H	-4.3427408883	0.2020110825	3.0436786867
H	-2.5531783956	-1.555552007	-1.1810159121
H	-4.4877069578	-0.3608681408	-2.1043726621
H	-3.8144852704	1.1891163742	-1.5401469197
H	-5.3020457999	-0.8998194091	0.1406143798
H	-5.3879939734	0.8755617747	0.2544694027
C	1.2114324609	-1.7891967655	-0.0820301158
C	0.8200269129	-3.1006734369	0.1795676453
C	2.4774885423	-1.487430328	-0.5698323862
C	1.7263684766	-4.135107276	-0.0535319208
C	3.3736939282	-2.5323911357	-0.8081239184
C	3.003181758	-3.8538545523	-0.5497477679
H	-0.1800012864	-3.2977318166	0.5506579638
H	2.7488062367	-0.4551857346	-0.7478577115
H	1.4321848717	-5.1609896842	0.1461983441
H	4.3646691851	-2.3074426479	-1.190736354
H	3.7040884262	-4.6621148108	-0.7342256629
H	3.7040884262	-4.6621148108	-0.7342256629

TS 6-31G(d,p) 0012

E(RB3LYP) = -1488.74665915 A.U.

First frequency = -211.6497 cm^{-1}

O	3.4450403849	0.1792253791	0.5730194339
O	1.9192364757	1.0659388457	2.0106717026
O	0.9563118493	-1.064918948	-1.5244783787
O	0.1864618644	-0.9953631677	0.6823571872
O	-3.0402341032	-1.9653574449	-0.0332042264
O	-2.3816053651	-0.8249027218	1.8057388333
N	-0.9020536683	0.1207925078	-1.0269464144
N	-2.835207954	1.0952035699	-1.1124594194
C	1.9654696458	1.7282961673	-1.6325218429
C	2.413554431	0.8100660713	0.7078370653
C	1.4746622429	1.3649354995	-0.2580209621
C	0.8354946943	1.9026810899	1.882909604
C	0.108401481	2.4457885961	2.9259818692

C	0.5736087918	2.1873252868	0.5270981354
C	-0.4588909157	3.0762139928	0.2130278691
C	-1.2060987371	3.6473378442	1.2553792033
C	-0.9346877641	3.3306037145	2.5912702191
C	0.30601436	-0.499875036	-0.4349128041
C	-2.2714198727	-3.170999177	1.9240675613
C	-2.6245636325	-1.961144773	1.1084728205
C	-2.4688725553	0.4255858448	1.1175965942
C	-3.9362329788	0.9197687627	0.947849813
C	-4.0099076572	1.6388051105	-0.4192007723
C	-1.9774731327	0.4691884328	-0.3035834431
C	-1.1089353589	0.5354718033	-2.3404194447
C	-2.3216273094	1.1603470319	-2.3898770232
H	1.1353219083	1.9269049551	-2.316171612
H	2.5851317447	2.6341972088	-1.6094338995
H	2.5678989534	0.9191764605	-2.0493088372
H	0.3416254021	2.203476867	3.9571196337
H	-0.6758487689	3.3229505633	-0.8223129209
H	-2.0058327538	4.3441789532	1.0218089929
H	-1.5272960753	3.7765852492	3.3837752645
H	-1.1799762726	-3.2548754088	1.9311713492
H	-2.6077713552	-3.0589363692	2.9566998727
H	-2.704135058	-4.0618309257	1.4704249445
H	-0.389970358	0.3195794801	-3.1101602834
H	-2.8496290713	1.6177890806	-3.2099767237
H	-1.8780905078	1.1045325319	1.73115676
H	-4.229586379	1.575343573	1.76733355
H	-4.5888408248	0.0458561586	0.9433331837
H	-3.8918171237	2.7214719824	-0.3301058535
H	-4.9173783333	1.4176411145	-0.9817124525
C	2.0022218899	-1.9679707627	-1.3984016004
C	2.1396095705	-2.8816345573	-0.3494363657
C	2.896333653	-1.9683983749	-2.4718673743
C	3.2063732105	-3.7818734482	-0.3819370492
C	3.9503444239	-2.8801606237	-2.4921088737
C	4.1136198032	-3.7890991981	-1.4437024044
H	1.4391052599	-2.8710344927	0.47196206
H	2.7516823526	-1.254371448	-3.2757016104

H	3.3219375452	-4.4883982487	0.4348679743
H	4.6445763978	-2.8759384115	-3.3270604282
H	4.9369332346	-4.4964624736	-1.4554503533
H	4.9369332346	-4.4964624736	-1.4554503533

TS 6-31G(d,p) 0016

E(RB3LYP) = -1488.75031527 A.U.

First frequency = -225.7892 cm^{-1}

O	-1.4177520889	2.1218715337	-0.5294948345
O	0.6709911688	1.6439331027	-1.3233821083
O	0.404187479	-0.844890841	0.374257379
O	0.6069908132	-0.300363179	2.6346604859
O	-3.5380946299	0.6265112073	-2.0385178306
O	-1.7003307845	-0.6955685483	-1.8528416219
N	-1.41447103	-0.1538373462	1.5050211062
N	-3.5064127531	-0.440996575	1.0085203702
C	0.0221262914	2.6758628087	2.1886901465
C	-0.2283506812	1.9654510171	-0.2709017716
C	0.4964934632	1.9492118503	0.9674090095
C	1.93134341	1.5541539143	-0.7765654346
C	3.0953476577	1.2768148342	-1.4686192545
C	1.8905753031	1.7821379236	0.6111708418
C	3.0826396862	1.7451960682	1.3379338538
C	4.2753137909	1.4673714995	0.6589485965
C	4.2827431568	1.2291050923	-0.7210037208
C	0.0653848011	-0.2089773834	1.5417957078
C	-1.6731010941	0.9196613389	-3.5578860424
C	-2.4278011683	0.3138525831	-2.4098981889
C	-2.2101328456	-1.4056433569	-0.7132871758
C	-3.6818379353	-1.9172299143	-0.8003665012
C	-4.5355633692	-1.02886044	0.13513116
C	-2.2595199428	-0.6048861916	0.5583015852
C	-2.169182017	0.3214435398	2.5672926527
C	-3.4868799932	0.147615503	2.2523910534
H	0.2928745169	2.1232277055	3.0964791652
H	0.4748949839	3.672646771	2.264652765
H	-1.0630984541	2.8044619752	2.1629103797

H	3.0832996753	1.0950838265	-2.5379819346
H	3.0785111833	1.9151667695	2.4102667937
H	5.2096481703	1.42778379	1.2117134535
H	5.2185658374	1.0064724486	-1.2246788088
H	-0.7339309919	1.3273017238	-3.1802199581
H	-1.4416368325	0.1489068791	-4.2987300018
H	-2.2761549887	1.705455848	-4.0111152873
H	-1.6938699614	0.7125138554	3.4491402492
H	-4.3819528274	0.3745109135	2.8072124664
H	-1.5069513859	-2.2298220713	-0.6102744293
H	-3.6975436503	-2.9488952324	-0.4415501974
H	-4.0469560128	-1.901831776	-1.8255513376
H	-5.2404214621	-1.598243567	0.7416884115
H	-5.0487145223	-0.2298414894	-0.3973785279
C	1.5868463892	-1.5304174773	0.1349981796
C	2.631826793	-1.6961303211	1.0437133509
C	1.6493143139	-2.0755378058	-1.151188465
C	3.7499419642	-2.4317017322	0.6412928157
C	2.7707650354	-2.8082311699	-1.5307696111
C	3.8277986744	-2.9924908518	-0.6339633267
H	2.5780635772	-1.2449009689	2.0221502868
H	0.8240447127	-1.8952870341	-1.8323827763
H	4.5705330103	-2.5593384594	1.3412424319
H	2.8200295954	-3.2299137171	-2.5302555236
H	4.704392912	-3.5602304919	-0.9298800747
H	4.704392912	-3.5602304919	-0.9298800747

TS 6-31G(d,p) 0017

E(RB3LYP) = -1488.74824334 A.U.

First frequency = -202.5997 cm^{-1}

O	3.4331441049	0.2885165772	0.5061304093
O	1.8241912144	0.8790954113	2.0062229993
O	1.1699475125	-0.8330447536	-1.6948377559
O	0.1620280551	-0.9774421789	0.4088454444
O	-1.9878823232	-1.2325059798	2.8826251332
O	-2.7747195305	-1.1726071223	0.7517463642
N	-0.7859842443	0.2427532727	-1.3104327607

N	-2.7609413276	1.1202061248	-1.5027380798
C	1.9261500415	2.077489983	-1.5057516858
C	2.372325958	0.8553052472	0.6998645675
C	1.444366803	1.5211033194	-0.1970966339
C	0.699700455	1.6690924297	1.9668829768
C	-0.0952981715	1.9960091194	3.0484673642
C	0.4720623354	2.1579130336	0.6628192315
C	-0.5977623994	3.0326895453	0.4484305848
C	-1.4078029938	3.3930613377	1.5368899271
C	-1.1716627745	2.8725935075	2.8134147947
C	0.3705097541	-0.3978818513	-0.65111100907
C	-2.3961737926	-3.2977691583	1.6831471107
C	-2.3505603944	-1.8082412878	1.8817742078
C	-2.5347089675	0.2459259542	0.6769692004
C	-3.8577190658	1.0529814805	0.5791565457
C	-4.0813881496	1.402194561	-0.9176336352
C	-1.9224109279	0.521674136	-0.6544727825
C	-0.9168487264	0.7032577124	-2.6172537123
C	-2.1623611167	1.2552869838	-2.7369446657
H	2.5413261964	2.9752121844	-1.3614525488
H	2.5297593587	1.3392103104	-2.0377147541
H	1.0890075631	2.3643070945	-2.1495655111
H	0.1084686019	1.594701913	4.0350785992
H	-0.7879465699	3.4392084661	-0.5409309295
H	-2.2327659938	4.0829570765	1.3838266141
H	-1.8174525708	3.1535059925	3.6394012023
H	-2.2654240782	-3.8026790085	2.639373964
H	-3.3359972719	-3.5980267253	1.2143685228
H	-1.581203721	-3.5746300982	1.0066902075
H	-0.1242345438	0.5785286071	-3.3334668404
H	-2.652959654	1.7127760874	-3.579935062
H	-1.9095706177	0.5551092126	1.5121663868
H	-3.7487416794	1.9668754029	1.163525494
H	-4.6831898054	0.4709737313	0.9891431033
H	-4.3400963071	2.4499169996	-1.07585228
H	-4.8264993739	0.7703055218	-1.4053289598
C	2.137808486	-1.817210952	-1.5276788211
C	1.9696598759	-2.9403971587	-0.714292375

C	3.2743376424	-1.6688153929	-2.3243875516
C	2.9767174615	-3.908238456	-0.6923156221
C	4.2641675582	-2.6490116396	-2.299080039
C	4.1223619874	-3.7716367972	-1.4784206776
H	1.0818086937	-3.0428313268	-0.1073748763
H	3.3671443474	-0.7885060739	-2.9507863056
H	2.8549306797	-4.7800045157	-0.0561534673
H	5.1485400865	-2.5316529796	-2.9180723553
H	4.8962687097	-4.5324533532	-1.4540036174
H	4.8962687097	-4.5324533532	-1.4540036174

TS 6-31G(d,p) 0018

E(RB3LYP) = -1488.75261369 A.U.

First frequency = -216.9248 cm^{-1}

O	-1.6877318503	2.4127360085	-0.2542135202
O	0.3173857297	2.1646067561	-1.3226469091
O	0.3056015187	-0.7020078375	0.1689196695
O	0.5517202814	-0.3850511239	2.4478751872
O	-0.8928482318	-2.2309159505	-2.3493109904
O	-1.5661585139	-0.1122625293	-1.877743202
N	-1.5073537769	-0.0569995955	1.4421611719
N	-3.6095281211	0.1683849166	0.9630517762
C	0.0259673198	2.5909024565	2.346366443
C	-0.4755961397	2.2484905401	-0.148931372
C	0.3666575986	2.0257051262	0.9982164935
C	1.6235998636	2.0113992992	-0.9232169926
C	2.7231983613	1.9550482322	-1.7630879054
C	1.7185823372	1.9523548318	0.4803284505
C	2.9789994967	1.8184850503	1.0665908767
C	4.106837882	1.7526708128	0.237162075
C	3.9838125858	1.8200451547	-1.1563396117
C	-0.0382326185	-0.1683742482	1.3995973277
C	0.306815055	-0.3594412049	-3.2913212847
C	-0.76157603	-1.0324595675	-2.481019154
C	-2.5447594721	-0.5972940226	-0.9736648016
C	-3.9409429296	-0.0360517469	-1.3357227432
C	-4.7128898224	0.0475447009	-0.0021651296

C	-2.4089483609	-0.108120461	0.4440571325
C	-2.1786058736	0.2799672445	2.6156222177
C	-3.5008548726	0.4153354669	2.3147455846
H	0.370866496	1.924927251	3.1456947976
H	0.5011921453	3.5677069484	2.500099238
H	-1.0541092677	2.7263204484	2.443924327
H	2.6106990236	2.0185420647	-2.8400938789
H	3.0792102081	1.763784288	2.1461223621
H	5.0921976536	1.6457500444	0.6812315474
H	4.8707067187	1.7677795708	-1.7803286662
H	0.5696457821	-0.9896495737	-4.1413766914
H	0.0011766659	0.6365232185	-3.6086516895
H	1.1855661498	-0.2510468311	-2.648715671
H	-1.6372560052	0.3892113942	3.5385404478
H	-4.3478385152	0.6584016303	2.9344951414
H	-2.5208554369	-1.6918248641	-0.9740476898
H	-4.4505122868	-0.651180816	-2.0770580566
H	-3.7853409486	0.9667959605	-1.7397041792
H	-5.2808626022	-0.8601995325	0.2166864087
H	-5.3729522792	0.9124114197	0.0692024966
C	1.2363066408	-1.7484738851	0.1760360543
C	2.5055605211	-1.5165055486	-0.3407719098
C	0.8461379914	-3.009072917	0.6235432862
C	3.4064377892	-2.5816757665	-0.416585004
C	1.7570824197	-4.0630280943	0.5514089782
C	3.0372487189	-3.8525255051	0.0294456332
H	2.7756344007	-0.52041386	-0.6658488002
H	-0.1564819312	-3.1535585398	1.0114540104
H	4.3999609684	-2.4113532709	-0.8202286495
H	1.4639134935	-5.0497810453	0.8967208196
H	3.7417741816	-4.6764066671	-0.0292928764
H	3.7417741816	-4.6764066671	-0.0292928764

TS 6-31G(d,p) 0020

E(RB3LYP) = -1488.74913816 A.U.

First frequency = -177.4490 cm^{-1}

O	-1.2636622774	1.296231413	2.6074390507
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O	-0.3707979099	2.8286692275	1.1655858755
O	1.4380305981	-0.7204224154	-0.365311494
O	-0.3526726854	-1.3471761625	0.9609776274
O	-2.370497865	-1.9920193776	-1.4313346817
O	-3.1438576045	-1.3905841706	0.6091065448
N	-0.5652167728	0.353869492	-0.598995496
N	-2.2761705407	1.3543378111	-1.4625163385
C	1.6008426387	0.0583763923	2.70560938
C	-0.2748535037	1.6540057833	1.9746791047
C	1.0149298471	1.0647232433	1.7624482688
C	0.8618179168	3.0264519865	0.5858508154
C	1.2030116146	4.0771674832	-0.246754367
C	1.7546428193	1.994504816	0.9434346656
C	3.0537489015	2.024623938	0.4233165763
C	3.41790334	3.0735494416	-0.4299235503
C	2.508990731	4.0875156137	-0.7621737503
C	0.2182621841	-0.5362480002	0.2525183738
C	-2.63096078	-3.6673853348	0.2958154279
C	-2.7027362873	-2.2924970126	-0.300306323
C	-3.0701171312	0.0004035445	0.2890989948
C	-4.262133121	0.4831304855	-0.5853814638
C	-3.7193494189	1.6384501536	-1.4574381029
C	-1.9032722259	0.4701745741	-0.5392721642
C	-0.0958689051	1.1838388029	-1.6160554076
C	-1.1759202572	1.8207298789	-2.1528592288
H	2.0357225207	0.5315512807	3.5954637847
H	0.828603497	-0.6419164994	3.0326259621
H	2.3923010142	-0.5195114417	2.2177275456
H	0.4824119254	4.8492020394	-0.4957395967
H	3.766499121	1.2468430263	0.6800869617
H	4.4237899498	3.1041994569	-0.8392468221
H	2.8147146742	4.8919751882	-1.4241845702
H	-2.639637424	-4.4141767121	-0.4976724432
H	-1.6823999703	-3.7276914387	0.8394611753
H	-3.4440172313	-3.8393413712	1.0027508518
H	0.9535337356	1.2399060022	-1.8449458041
H	-1.2467956186	2.5507758364	-2.9414004053
H	-3.0217988917	0.4990128013	1.258647059

H	-5.1106838465	0.7915793302	0.0244040186
H	-4.5671619723	-0.3486585476	-1.2228387671
H	-3.8826666889	2.6210946805	-1.0089001967
H	-4.1071144067	1.6374050727	-2.476431868
C	1.9627119137	-2.0127517717	-0.39169202
C	1.1987102393	-3.0933375736	-0.8371556369
C	3.3007296607	-2.1612206569	-0.0388145651
C	1.7969134181	-4.3516252217	-0.9076247885
C	3.8889969462	-3.4249271863	-0.1249045772
C	3.138555933	-4.5224866776	-0.5523762474
H	0.1630498125	-2.9452868418	-1.1220960924
H	3.8611633911	-1.2930856343	0.2901475228
H	1.2115685379	-5.2001161262	-1.2487893333
H	4.9327626716	-3.5485979481	0.1467851563
H	3.5961524405	-5.5049176258	-0.6123655835
H	3.5961524405	-5.5049176258	-0.6123655835

TS 6-31G(d,p) 0021

E(RB3LYP) = -1488.74857708 A.U.

First frequency = -21.7886 cm^{-1}

O	-0.8964828263	3.084637774	-0.0292182574
O	1.3868201189	2.7531175931	-0.0181095558
O	0.8958458713	-0.150569815	-1.3703773381
O	-0.333720966	-1.3206613114	0.1756044636
O	-2.6237953852	-2.1820614844	2.3164888989
O	-3.1393132274	-1.9605865338	0.1135430758
N	-1.2810300065	0.3273770542	-1.1440829726
N	-3.2981675511	1.0532206632	-1.437587375
C	-0.9567194792	1.1286314102	2.4214162506
C	0.0613702516	2.5200899716	0.5211894612
C	0.1847728434	1.6254134068	1.5970830437
C	2.2630932327	2.0432087917	0.7536704224
C	3.6350763139	1.9887421898	0.5973160462
C	1.5705697911	1.3454959072	1.7788702757
C	2.3187771262	0.5828903297	2.6919054681
C	3.711838274	0.5255536815	2.5476522695
C	4.3651555973	1.2084737566	1.5140373107

C	-0.1879905734	-0.4604764483	-0.6557938362
C	-2.2774453526	-4.0396328119	0.7998998086
C	-2.6873837557	-2.6533016225	1.2037416674
C	-3.3643822995	-0.5586317702	0.2802553898
C	-4.8141413099	-0.1794901089	-0.1380321846
C	-4.7122005503	1.0827908063	-1.0289454611
C	-2.558991051	0.2232348158	-0.7124754348
C	-1.2459510618	1.2762180003	-2.1699938668
C	-2.5174501314	1.724592594	-2.3550862971
H	-0.8559527878	1.3894085592	3.4844100801
H	-1.8913367562	1.5745420314	2.0645809842
H	-1.0549078295	0.0350399742	2.3716845614
H	4.1255627309	2.5297364807	-0.2062660048
H	1.8225278696	0.0439168631	3.4945458209
H	4.2961000366	-0.0659513631	3.2481235041
H	5.4446663677	1.141244946	1.4170322489
H	-1.3202934148	-3.9625639268	0.2744287724
H	-2.1582018407	-4.6616185939	1.6860024913
H	-3.0055832342	-4.4778181366	0.1142820456
H	-0.3213274022	1.53900178	-2.6509857175
H	-2.9126504108	2.4657195713	-3.0288450052
H	-3.1264192263	-0.2735382362	1.3052732075
H	-5.4534706363	-0.0153712363	0.7287762019
H	-5.2161133971	-1.0140807926	-0.7162424036
H	-4.8935688457	2.0078612086	-0.4780561817
H	-5.3551920815	1.0531572636	-1.9085205655
C	2.0252505311	-0.9978863983	-1.3578874039
C	2.6434881246	-1.385183572	-0.1765341529
C	2.5098730146	-1.3577220689	-2.611329373
C	3.7892841164	-2.1776864548	-0.2655496697
C	3.6589623291	-2.1466959579	-2.6812226686
C	4.2975919272	-2.5603461665	-1.5089532948
H	2.2585172127	-1.0554881593	0.7778857243
H	1.9931269434	-1.0212221948	-3.5034392287
H	4.2903460563	-2.481212316	0.6480782743
H	4.0513544477	-2.4357208691	-3.6510126496
H	5.192271722	-3.1724022274	-1.5656538664
H	5.192271722	-3.1724022274	-1.5656538664

TS 6-31G(d,p) 0026
E(RB3LYP) = -1488.74972912 A.U.
First frequency = -177.2108 cm⁻¹

O	3.5483989233	0.6456509678	0.8542053118
O	1.8204351777	1.176781569	2.2442414847
O	1.5010110318	-0.6254592679	-1.3839807214
O	0.3618180264	-0.7835748431	0.6260971886
O	-2.3349745977	-2.0526448878	-0.7578488765
O	-2.3244740639	-1.0582237906	1.2754400817
N	-0.5585534261	0.3740834367	-1.144331503
N	-2.5563897855	1.143051418	-1.4715944403
C	2.0975694759	2.3384185867	-1.2732173024
C	2.4532339367	1.1715886267	0.9756717061
C	1.5634951202	1.7960775335	0.0211031772
C	0.6609650242	1.9053342446	2.1229949374
C	-0.2307027642	2.1830400614	3.141682351
C	0.5005245485	2.381516162	0.8039058994
C	-0.6054343122	3.1860941823	0.5075112971
C	-1.5171839777	3.4912540569	1.5297814964
C	-1.3404859406	2.9898926756	2.8249655801
C	0.5852893914	-0.2104258716	-0.4316454236
C	-1.7235930744	-3.33461019	1.200805171
C	-2.1713827226	-2.1181166585	0.4459699241
C	-2.4822011215	0.2458881323	0.7072726719
C	-3.9558279863	0.5500634142	0.3064936185
C	-3.8959121636	1.448214069	-0.9510892453
C	-1.7685502236	0.5305756529	-0.5854677832
C	-0.6031268904	0.8928477097	-2.4355176946
C	-1.8583347185	1.3906519694	-2.635206891
H	2.6393843415	1.5638265375	-1.8223053317
H	1.2893549565	2.7104946252	-1.9094973408
H	2.787277566	3.1761511885	-1.1070623198
H	-0.0735216144	1.7981144273	4.1435542305
H	-0.7498767655	3.5752168316	-0.4964733964
H	-2.3746569485	4.1213963444	1.3115412817
H	-2.0605711909	3.2305858375	3.600761083
H	-0.6343281417	-3.2640472756	1.2888737708

H	-2.1505537678	-3.3639255885	2.2042481898
H	-1.9805181681	-4.2330446848	0.6401095399
H	0.2520846576	0.8368289992	-3.0851155599
H	-2.3003407976	1.8740658937	-3.4904635108
H	-2.1185953929	0.9199392322	1.4842524251
H	-4.5026037212	1.023450878	1.1215208393
H	-4.4376641007	-0.3979618544	0.0614848893
H	-3.9455013324	2.513020632	-0.7102010657
H	-4.6552442385	1.2093811838	-1.6961171482
C	2.0114650019	-1.9175831147	-1.2132728
C	1.16299941	-3.0177917012	-1.34069703
C	3.3728830942	-2.0624648687	-0.9745830494
C	1.7058141225	-4.2987890392	-1.2329658628
C	3.9050680891	-3.3510237774	-0.8825547084
C	3.076158883	-4.4683122723	-1.011326125
H	0.1014890391	-2.8644274656	-1.5074492046
H	3.9753961783	-1.1729145257	-0.833337036
H	1.0568283619	-5.1644006121	-1.3263853211
H	4.9675001777	-3.4792368331	-0.6985647703
H	3.4939207751	-5.4673286473	-0.9329811948
H	3.4939207751	-5.4673286473	-0.9329811948

TS 6-31G(d,p) 0027

E(RB3LYP) = -1488.74768329 A.U.

First frequency = -164.8348 cm^{-1}

O	1.0338169411	0.4340039736	-2.7313428402
O	2.5688346714	1.4304838976	-1.3808846187
O	0.1005899075	-0.9980279777	-0.2715028752
O	1.4928883608	0.1184022421	1.2118941306
O	-1.9931037337	-3.0563150986	-1.297539404
O	-2.630254951	-0.8865006556	-1.0781141171
N	-0.8084690547	0.3996912897	1.3195446655
N	-2.8466104731	0.5721524158	2.0360453415
C	-1.0842317914	2.0395970543	-1.166721
C	1.2405726577	1.1435417976	-1.7571202528
C	0.3463007201	1.7628699628	-0.7971204704
C	2.5145132766	2.3803796885	-0.3811231139

C	3.6069060122	2.9991650393	0.1988930334
C	1.1828252132	2.6896162083	-0.0525884342
C	0.9369229348	3.6867837999	0.8937169414
C	2.0265089283	4.3302190083	1.4964405369
C	3.3416833664	3.9867192669	1.1606561536
C	0.4462958448	0.0564743848	0.5801658187
C	-1.7180351933	-1.5163640161	-3.1510003445
C	-2.1131676421	-1.9494632968	-1.7723310906
C	-2.8262326419	-1.0455837672	0.3241391222
C	-4.2929490808	-0.7023444504	0.7053225946
C	-4.2353750009	0.0848500496	2.0349602547
C	-2.0665975561	-0.0284137325	1.1291597547
C	-0.807719313	1.2974197269	2.3769687239
C	-2.0915085625	1.403161066	2.8346049867
H	-1.5721638469	1.1447472644	-1.5546927328
H	-1.652835206	2.3877725795	-0.2977808645
H	-1.1553217324	2.8235810877	-1.931236483
H	4.6193861467	2.7337444934	-0.0858291191
H	-0.080931743	3.962032664	1.1538267158
H	1.8483110186	5.1098920801	2.2313274821
H	4.171269538	4.4969165624	1.6407260245
H	-0.8395554221	-0.8663481363	-3.0589669348
H	-1.4776412383	-2.3901305865	-3.7555408487
H	-2.5198879649	-0.9372624677	-3.6156823383
H	0.1091643079	1.7682158276	2.6860462355
H	-2.5129964062	1.9824506036	3.6392026815
H	-2.5334784583	-2.058110411	0.6136109962
H	-4.91170105	-1.5958785742	0.7834024348
H	-4.6941563338	-0.0676313748	-0.088043614
H	-4.3852222822	-0.5509777057	2.9103444928
H	-4.9298653333	0.9243311862	2.0767606608
C	0.9439417244	-2.1126521306	-0.2633261361
C	0.9945994673	-2.9351256934	0.8617110931
C	1.6572921895	-2.4139442027	-1.4187326129
C	1.7788864363	-4.087894514	0.823433612
C	2.4323839606	-3.5761057066	-1.4480797126
C	2.4969713689	-4.4127694198	-0.3315713563
H	0.4236393473	-2.6710788936	1.745415484

H	1.6032860174	-1.7315441213	-2.2589236217
H	1.8243375774	-4.7347667232	1.6944796315
H	2.9913654281	-3.822782953	-2.3459132796
H	3.1037537146	-5.3127012176	-0.3589708717
H	3.1037537146	-5.3127012176	-0.3589708717

TS 6-31G(d,p) 0028

E(RB3LYP) = -1488.74719868 A.U.

First frequency = -178.5349 cm^{-1}

O	1.3022775212	0.3423007762	-2.5312790824
O	2.7277283797	1.3662971767	-1.0847293337
O	0.1137053389	-1.0556961983	-0.1673554238
O	1.3448382308	0.0932903175	1.4356511531
O	-2.3035713255	-2.9733084254	-1.6951380373
O	-2.5055397841	-0.7408586824	-1.3520738976
N	-0.9500682123	0.3851849847	1.2711397194
N	-3.0502765723	0.6281454869	1.75214048
C	-0.9074941319	2.0610362233	-1.2080157429
C	1.427518314	1.0781529169	-1.5677857845
C	0.461459489	1.7159533076	-0.6875840479
C	2.5967681685	2.3182100257	-0.0925172621
C	3.6421505487	2.9286996888	0.575883896
C	1.2460900699	2.6346652133	0.1256180217
C	0.9285326251	3.6310687546	1.0499953053
C	1.9684845255	4.2670388881	1.7422348095
C	3.3044419466	3.916260418	1.5147721827
C	0.3835564623	0.0299246768	0.6779138746
C	-1.5142235408	-1.4061849788	-3.3734969583
C	-2.1400022867	-1.8365052679	-2.0816746722
C	-2.8959715222	-0.9394646133	0.0039412574
C	-4.3815143612	-0.5344599096	0.2163040983
C	-4.4490119925	0.2090827006	1.5700754523
C	-2.1930360974	0.0130388022	0.9279531761
C	-1.0393751016	1.2640885228	2.3405921092
C	-2.3625185933	1.4131424288	2.6506442905
H	-1.5663218926	2.3875809742	-0.396302876
H	-0.858254429	2.8861825839	-1.9296864604

H	-1.3717287179	1.2071271823	-1.6994758553
H	4.6729691329	2.6573263249	0.3748811392
H	-0.1058100532	3.9107270774	1.2268653224
H	1.7349823333	5.045646644	2.4625436865
H	4.0948194196	4.4200142538	2.0629552189
H	-0.5785442542	-0.8830290211	-3.1432269333
H	-1.3227785265	-2.2780732102	-3.9975512332
H	-2.1693861964	-0.702256121	-3.8937071869
H	-0.1473191821	1.6927125684	2.7631405117
H	-2.8520316722	1.9940249275	3.4145060413
H	-2.6964116187	-1.9748751272	0.2894599248
H	-5.0454758648	-1.3980296857	0.1867855411
H	-4.6520831244	0.1431833887	-0.5966359012
H	-4.7311102863	-0.444637712	2.3984127999
H	-5.1051786681	1.0796782346	1.5589325369
C	1.0309463722	-2.1051236853	-0.2241067434
C	0.4873672239	-3.3892606982	-0.180581721
C	2.4060546707	-1.9112897828	-0.3745950634
C	1.329025226	-4.4966497358	-0.2985428862
C	3.2353958053	-3.029177571	-0.4789257088
C	2.7065814018	-4.3220258853	-0.4437774399
H	-0.584075166	-3.507482865	-0.0776560453
H	2.8153159972	-0.9122115827	-0.4067851703
H	0.9029600109	-5.4952725336	-0.271626243
H	4.3054278693	-2.8828197784	-0.5945749805
H	3.3616335369	-5.1834447886	-0.5314625898
H	3.3616335369	-5.1834447886	-0.5314625898

TS 6-31G(d,p) 0030

E(RB3LYP) = -1488.74981740 A.U.

First frequency = -223.3558 cm^{-1}

O	-0.9649333998	1.530457453	2.4830492259
O	-0.1868370813	2.8758084922	0.8237855784
O	1.1482370914	-0.8069675811	-0.7909859156
O	-0.2583713409	-1.3891165239	0.9819067604
O	-3.9010413465	-1.4603433882	-1.3618256598
O	-3.2647110633	-1.6265117067	0.8055777053

N	-0.8476696517	0.2223993155	-0.5719601262
N	-2.7287022025	1.233591289	-0.9315874793
C	1.8148028176	0.1608729155	2.3575258843
C	-0.0663417221	1.7550129614	1.6836990305
C	1.1295386229	1.0175319277	1.3266253042
C	0.9650384559	2.9377934123	0.067033606
C	1.2592205305	3.9157754837	-0.8668534213
C	1.8223629346	1.8635610151	0.367268374
C	3.0473702076	1.7798494002	-0.2998051581
C	3.3688858226	2.7556163057	-1.251083404
C	2.4876221788	3.807277792	-1.5361712481
C	0.1604137293	-0.5811231427	0.1585407576
C	-3.82669753	-3.6301903817	-0.2841139371
C	-3.6867814617	-2.1348156726	-0.3736214228
C	-2.9972134613	-0.2111456113	0.9220839095
C	-4.2461132063	0.7064684949	0.7743696136
C	-4.1513326414	1.403855492	-0.6066227334
C	-2.1133006579	0.3499298013	-0.1468655191
C	-0.6753345668	1.044154725	-1.680305674
C	-1.866551298	1.6771693701	-1.9082432564
H	2.6410804659	-0.3999194264	1.9132114729
H	2.2194971054	0.7657889589	3.1783744356
H	1.1073299145	-0.5591036098	2.7754866644
H	0.5649480184	4.7246671797	-1.0679453957
H	3.7327279395	0.9655573431	-0.0896220674
H	4.3177742331	2.6969112259	-1.7764919254
H	2.7565794066	4.551353688	-2.2796596096
H	-2.8431207775	-4.0719185208	-0.098701441
H	-4.4719270759	-3.8982285225	0.556379848
H	-4.2382539817	-4.0153933878	-1.21593214
H	0.2746955555	1.1119214936	-2.1792398593
H	-2.1502932411	2.3971512088	-2.6575260808
H	-2.5216906645	-0.1231978204	1.8942497402
H	-4.2089520455	1.4548126406	1.5684199384
H	-5.1658456853	0.1316687409	0.8831521189
H	-4.3999556771	2.4648172498	-0.5703851411
H	-4.7430694218	0.9026859457	-1.3731150021
C	2.2012700079	-1.6886653845	-0.6106124508

C	3.2868440612	-1.4587118597	-1.4624361852
C	2.2105343194	-2.7625920545	0.2852686381
C	4.3942667491	-2.3023468605	-1.4148163281
C	3.3343697953	-3.592638916	0.324898463
C	4.4258507745	-3.3731072708	-0.5166554936
H	3.2466146772	-0.613329904	-2.1402671691
H	1.3649825917	-2.9317474459	0.9346048821
H	5.2345067686	-2.1177184392	-2.0773481709
H	3.3465176595	-4.4237013427	1.024018481
H	5.2905807494	-4.0278095798	-0.4747488159
H	5.2905807494	-4.0278095798	-0.4747488159

TS 6-31G(d,p) 0036

E(RB3LYP) = -1488.74679512 A.U.

First frequency = -212.7442 cm^{-1}

O	2.2322927764	-0.0958781347	2.7213657968
O	0.5744010425	1.4466967929	2.6073971101
O	1.594690119	-1.156817643	-1.0052651448
O	0.1441315208	-1.249963358	0.8142772747
O	-3.5680597201	-1.2099520643	-1.2789353419
O	-2.8467471867	-0.9206997039	0.8484673727
N	-0.2815195305	0.1204819718	-1.0105805707
N	-2.0173550805	1.2882364617	-1.5774396729
C	3.1117513292	0.988319331	-0.041273905
C	1.6409980666	0.7142508389	2.0372982495
C	1.7551746453	1.063861338	0.6182158045
C	0.1846629229	2.391049298	1.679503418
C	-0.7814030148	3.3598534689	1.8841533741
C	0.9108655559	2.2547447773	0.4834920117
C	0.6840229583	3.1730569646	-0.5429198852
C	-0.2924402748	4.1637731361	-0.3655758086
C	-1.0223319083	4.251377092	0.8244919815
C	0.6618604009	-0.613899649	-0.1027493721
C	-3.7091930763	-3.0369161569	0.3081678408
C	-3.3901378516	-1.6428793825	-0.1574306046
C	-2.3731492405	0.4182587111	0.5921898922
C	-3.4845231022	1.4505519721	0.242457295

C	-3.3727797237	1.7613843233	-1.2713121568
C	-1.4795311724	0.5524229352	-0.6023177951
C	-0.0652183095	0.5981329216	-2.2937380068
C	-1.167608178	1.3258707809	-2.655877885
H	3.6304460495	0.0724499978	0.2482916652
H	3.0178417731	0.9869688407	-1.1304250493
H	3.7384828301	1.8425727076	0.2431580437
H	-1.3172664239	3.4283428454	2.8246680689
H	1.2458725965	3.1137615934	-1.4690393109
H	-0.4828149965	4.8751687727	-1.163452688
H	-1.7745411655	5.0251589227	0.9421804803
H	-4.3104332726	-3.0035713726	1.2200628327
H	-4.2389407181	-3.5732076341	-0.4778450621
H	-2.7744380607	-3.5526849189	0.5476543703
H	0.8456466937	0.3794721011	-2.8227740667
H	-1.3941589419	1.8606777505	-3.5631529574
H	-1.8480761468	0.6660686668	1.5109701551
H	-3.2920719284	2.3581921155	0.8173824568
H	-4.4675708601	1.0659100716	0.5135436974
H	-3.4517777568	2.8255036449	-1.4948796399
H	-4.0830852227	1.1929726339	-1.8722410847
C	2.3041646993	-2.2995599166	-0.6803791515
C	2.6098004123	-3.1334695529	-1.7590936417
C	2.7585547657	-2.5936531662	0.6082453915
C	3.3784854815	-4.2780137965	-1.5489746091
C	3.519820216	-3.7491639563	0.8014094183
C	3.8341338358	-4.5932694899	-0.2660880315
H	2.2405967656	-2.8726889483	-2.7455770292
H	2.5245941043	-1.9323043232	1.4324646006
H	3.6161915661	-4.9239996601	-2.3889969839
H	3.8745328643	-3.9838330077	1.8009467219
H	4.4300524097	-5.4856568741	-0.1013075616
H	4.4300524097	-5.4856568741	-0.1013075616

TS 6-31G(d,p) 0039

E(RB3LYP) = -1488.75031529 A.U.

First frequency = -225.7951 cm^{-1}

O	-1.2475806834	2.0696887247	-0.9348961782
O	0.8232890284	1.3295207352	-1.5554972369
O	0.3404020432	-0.8047693441	0.5323117561
O	0.520959554	0.1098158591	2.6719273677
O	-3.4259502884	0.4737476346	-2.2444800291
O	-1.6896219794	-0.9103233193	-1.7656558435
N	-1.4551401532	0.1863649187	1.4582685214
N	-3.5481845053	-0.0487660316	0.9395544607
C	0.1551271992	2.9945505528	1.7005311521
C	-0.0790349099	1.8853205478	-0.6085185657
C	0.6101225498	2.0382708353	0.640776423
C	2.0596075999	1.2561401296	-0.9540839538
C	3.2194511163	0.789466657	-1.5437794183
C	1.9982150437	1.7236907098	0.371466214
C	3.1653506454	1.7378181868	1.1383828914
C	4.353409594	1.271124329	0.5627174811
C	4.3806348688	0.7969224285	-0.7546612823
C	0.0158623054	0.0444196633	1.5598789907
C	-1.5059171046	0.3795497217	-3.7200015836
C	-2.3306013798	0.031361511	-2.5145476832
C	-2.2770735919	-1.3779277011	-0.5413534083
C	-3.7778810436	-1.8021133942	-0.5950821627
C	-4.592291133	-0.7124083345	0.1414564084
C	-2.304242781	-0.3672419291	0.5714734746
C	-2.2027637287	0.8856930249	2.3941618247
C	-3.5206119463	0.7441318872	2.0641016018
H	-0.9175787191	3.1853109627	1.6120680403
H	0.3631399837	2.5918769989	2.6992179183
H	0.6734676008	3.9586161317	1.621488318
H	3.2229968814	0.4259871692	-2.5658251059
H	3.1447775855	2.0912729127	2.164760522
H	5.2679125921	1.2688113299	1.1490410478
H	5.3117500754	0.4312197068	-1.1769215267
H	-0.5512498088	0.7864394095	-3.3825143535
H	-1.3085019849	-0.5212530872	-4.3082721096
H	-2.0412650041	1.1111719194	-4.323900738
H	-1.72482504	1.3926661302	3.2133483942
H	-4.4120868974	1.1202801285	2.5376504612

H	-1.6356131899	-2.2148139927	-0.2720964069
H	-3.8743999667	-2.7527911055	-0.0657183779
H	-4.114021444	-1.9415235181	-1.6208149952
H	-5.3506182788	-1.1218666197	0.8094504832
H	-5.0346454788	0.0131981228	-0.5390858371
C	1.4786896945	-1.5952201683	0.4590574542
C	2.4855053155	-1.6667140371	1.4215642062
C	1.5370656758	-2.3582410112	-0.7112969535
C	3.5602882214	-2.5305123109	1.1937850341
C	2.6147680533	-3.2154659306	-0.916955537
C	3.6326429375	-3.3080001316	0.0374552194
H	2.437392124	-1.0499886898	2.3054015529
H	0.7443999475	-2.2469283072	-1.444012394
H	4.3514435654	-2.5865529144	1.935757402
H	2.6609764162	-3.8065521275	-1.8267341345
H	4.4753656348	-3.9730289838	-0.1233780601
H	4.4753656348	-3.9730289838	-0.1233780601

TS 6-31G(d,p) 0040

E(RB3LYP) = -1488.74725363 A.U.

First frequency = -208.3053 cm^{-1}

O	1.9238677507	-0.3432847279	2.6102321897
O	0.3011143164	1.2386269918	2.5079445988
O	1.5766259481	-1.0640923286	-1.2315967257
O	-0.0084691198	-1.3018335214	0.4536964859
O	-2.8042248854	-1.3010007038	2.2721910248
O	-2.9711786538	-0.9199574941	0.0391381588
N	-0.2788666051	0.2376823569	-1.2620812639
N	-1.9825197216	1.4377003136	-1.8624512295
C	3.0355788559	0.973967186	0.0285233326
C	1.4039395887	0.5415860176	1.9595704102
C	1.6388525432	1.0211463501	0.5981791453
C	-0.0087942661	2.2634349744	1.6392709738
C	-0.9834051983	3.222368256	1.8494055986
C	0.8102743818	2.2221734845	0.4963594095
C	0.660636355	3.2205949289	-0.4685214309
C	-0.3248401326	4.2011344221	-0.2851422672

C	-1.1402241489	4.200102385	0.8517593844
C	0.5780095374	-0.5984343092	-0.3677076616
C	-3.1668776724	-3.1531489467	0.7538416088
C	-2.9668056891	-1.7169915795	1.1471597577
C	-2.4677455968	0.4193476675	0.2076582877
C	-3.5410646987	1.4933478734	-0.1073537664
C	-3.3528457192	1.9024469334	-1.5924447997
C	-1.4928041565	0.6592424188	-0.8951074983
C	0.0126433799	0.7897993521	-2.5006891132
C	-1.0677832396	1.5386803738	-2.8854120509
H	3.0174761945	1.055886146	-1.061615812
H	3.6510339897	1.7943497705	0.4183554213
H	3.5240278643	0.0310450406	0.2815526561
H	-1.5909254791	3.216866974	2.7478840912
H	1.2900796704	3.2312883057	-1.352263992
H	-0.4541419017	4.9754953125	-1.0352827351
H	-1.8964751124	4.9689700931	0.9758407807
H	-2.221396808	-3.5133458464	0.3349643872
H	-3.4259249104	-3.745486549	1.6305541177
H	-3.9343743373	-3.2459945288	-0.0173167773
H	0.9512547724	0.5969187761	-2.9899241055
H	-1.2423613804	2.1226883992	-3.7736855189
H	-2.0362217027	0.5175457899	1.2008781746
H	-3.3592484631	2.3576970032	0.533673506
H	-4.5406254917	1.1071306387	0.0916831598
H	-3.4161733879	2.9795268581	-1.7487892164
H	-4.0402385219	1.3954388839	-2.272881483
C	2.2594339985	-2.2365805698	-0.9496230448
C	2.6166023631	-2.6354219099	0.3409783678
C	2.6412944066	-2.9817029025	-2.0675930281
C	3.3594709575	-3.8086497101	0.4949036784
C	3.390112537	-4.1456369829	-1.8949913763
C	3.7494165145	-4.5663348982	-0.6118178269
H	2.3243604134	-2.0399513072	1.1965509111
H	2.3463232738	-2.6391620945	-3.0540249432
H	3.6395314405	-4.1258146364	1.4953000187
H	3.6878012523	-4.7237849329	-2.7647382393
H	4.329961327	-5.4736865295	-0.476634524

H 4.329961327 -5.4736865295 -0.476634524

TS 6-311++G(d,p) 0008

E(RB3LYP) = -1489.12290032 A.U.

First frequency = -233.1518 cm^{-1}

O	-1.7379126748	2.5489114375	0.2869608716
O	0.03272422	2.2758582456	-1.1130426188
O	0.3777411167	-0.6512335485	0.2934480272
O	0.764355888	-0.3550815836	2.5589346566
O	-0.8757276448	-1.8018086251	-2.7298789486
O	-1.9623666502	-0.1624205645	-1.6131717548
N	-1.3604179704	-0.0829850555	1.6675680551
N	-3.4852534874	-0.1929814857	1.2644978211
C	0.4086524697	2.5981564275	2.5496774267
C	-0.5412825464	2.3338038227	0.1819921502
C	0.4836146509	2.046399968	1.1547415396
C	1.3867672229	2.0888564781	-0.9581045398
C	2.3158315346	2.0511763906	-1.979539178
C	1.7218275438	1.9732388237	0.400342274
C	3.0613133708	1.8035563658	0.7499413945
C	4.0224822158	1.7519548312	-0.266308688
C	3.6583984184	1.8741250426	-1.6107468509
C	0.1136710657	-0.1393028008	1.5523365123
C	-0.9579745519	0.4286546649	-3.657147949
C	-1.226868476	-0.6479269666	-2.6485255469
C	-2.343634337	-1.0920004223	-0.5852976037
C	-3.8527940749	-1.4503417678	-0.6715303517
C	-4.584231581	-0.549593088	0.3515847642
C	-2.2779065114	-0.4243509617	0.7496894869
C	-2.0271325963	0.3792967171	2.7923214832
C	-3.3655313887	0.3163887723	2.5371406502
H	-0.627012973	2.7835133931	2.8396624066
H	0.8575195694	1.9060727716	3.2685275799
H	0.9477501552	3.5495139371	2.6221541165
H	2.017950648	2.1540354366	-3.0158460823
H	3.3512522873	1.7102528909	1.7901722177
H	5.066532851	1.6147330516	-0.0079402273

H	4.4194632829	1.8323692011	-2.3813946378
H	-0.1718862217	0.103589024	-4.3356607632
H	-1.874168736	0.6083011727	-4.2269466242
H	-0.6852056681	1.3531381272	-3.1513574167
H	-1.4862521842	0.6932814549	3.6655177544
H	-4.2128778785	0.5765154473	3.1463586561
H	-1.7001582106	-1.9660609884	-0.6394926738
H	-3.9805588297	-2.4978540821	-0.3969779908
H	-4.2213664083	-1.3107378094	-1.6858840409
H	-5.3697112941	-1.068361144	0.8970526767
H	-4.9873383732	0.3633514603	-0.0875704054
C	1.3660819385	-1.6264435147	0.1499215645
C	1.365515168	-2.7812918555	0.9283986645
C	2.290684515	-1.439636592	-0.868975338
C	2.325529017	-3.7613091289	0.6798274388
C	3.2398770307	-2.4302808317	-1.114047985
C	3.2632988443	-3.5908865616	-0.3400291676
H	0.6333177222	-2.9061684997	1.7151603026
H	2.2606413983	-0.5277216552	-1.4482880205
H	2.3349280244	-4.6620643788	1.2829730083
H	3.9641543193	-2.2893960751	-1.9082354728
H	4.0051559566	-4.3579217303	-0.5297723059
H	4.0051559566	-4.3579217303	-0.5297723059

TS 6-311++G(d,p) 0016

E(RB3LYP) = -1489.11972959 A.U.

First frequency = -255.6951 cm^{-1}

O	-1.3690039976	2.2152556871	-0.5422360839
O	0.711406383	1.7159802195	-1.3146225571
O	0.4161102162	-0.7851153348	0.3365241059
O	0.604375549	-0.2914756779	2.6027062864
O	-3.5360850352	0.6271362208	-2.0062031018
O	-1.7028491041	-0.6889618908	-1.8626221573
N	-1.4175582333	-0.1214358932	1.4761215939
N	-3.5012372334	-0.4825669095	1.0009770005
C	0.0455059367	2.6995659029	2.2001486232
C	-0.1953241735	2.0213509026	-0.2687204797

C	0.5103055398	1.9566057253	0.9833982822
C	1.965488193	1.6038669099	-0.7556144191
C	3.1347276758	1.3398196585	-1.4392822644
C	1.9097297008	1.7986321329	0.6330554276
C	3.0921270731	1.7586249203	1.3706593103
C	4.2923812931	1.5003887361	0.7001625728
C	4.3135924153	1.2836911847	-0.6810409903
C	0.0730619433	-0.1585539811	1.5129330124
C	-1.7076289089	0.9292818234	-3.5621014362
C	-2.4381254698	0.3192528294	-2.4039249369
C	-2.1925244591	-1.4175283939	-0.7206979335
C	-3.6494286797	-1.9623079828	-0.8089145894
C	-4.5200750592	-1.107461946	0.1404946044
C	-2.254884618	-0.6185223996	0.5481777533
C	-2.1798696549	0.348581867	2.5345865092
C	-3.4917224778	0.1285469504	2.2334235417
H	0.324409164	2.1593298098	3.1103869614
H	0.5043856717	3.693383198	2.2535187613
H	-1.0372302047	2.8343573817	2.1871738699
H	3.1370059683	1.1798794195	-2.5105072286
H	3.0775873519	1.9115430306	2.4435476277
H	5.2199199047	1.4566214644	1.260176552
H	5.2534680356	1.0721697989	-1.177916317
H	-0.729646928	1.2714214727	-3.2238062145
H	-1.5596855137	0.1750585207	-4.3390507525
H	-2.2859356565	1.7614492344	-3.9573622923
H	-1.7165071142	0.7698136493	3.4069349908
H	-4.3880455941	0.3388161281	2.7895374985
H	-1.4715427799	-2.2237344659	-0.6260179749
H	-3.6382962045	-2.9972794574	-0.4655599375
H	-4.0179549992	-1.9431196094	-1.8312105824
H	-5.1918469062	-1.7046138391	0.7546241156
H	-5.0728019877	-0.328729688	-0.3790618892
C	1.5688005548	-1.5227911376	0.1117238959
C	2.6294330115	-1.6715498881	1.0018292127
C	1.593936217	-2.1286168447	-1.1466282595
C	3.7180153323	-2.4559574788	0.6156483462
C	2.6874644641	-2.9050900356	-1.5138080396

C	3.7560291211	-3.0769118795	-0.6310260029
H	2.6143643244	-1.1728498796	1.9566119172
H	0.7624642051	-1.9643093127	-1.8214340977
H	4.5484513317	-2.5702314337	1.3034152476
H	2.7057463082	-3.3715886838	-2.4922995579
H	4.6103450513	-3.679462354	-0.9165275724
H	4.6103450513	-3.679462354	-0.9165275724

TS 6-311++G(d,p) 0017

E(RB3LYP) = -1489.12159437 A.U.

First frequency = -203.9372 cm^{-1}

O	3.6328326128	1.019822306	0.2813203528
O	2.0528088806	1.3868335798	1.8691859409
O	1.5064813681	-0.4904758528	-1.6387494679
O	0.5021289747	-0.6761497312	0.4392927304
O	-1.715262085	-1.2849585656	2.9218106872
O	-2.3839659196	-1.3035266853	0.7608244959
N	-0.6191617551	0.3471439574	-1.2988553156
N	-2.7000724869	0.9213717512	-1.4982364804
C	1.7583093435	2.5207289533	-1.6474661794
C	2.5136442753	1.4206328746	0.5364839052
C	1.4453720551	1.922551322	-0.305507745
C	0.8234823977	2.0060267674	1.8994370228
C	0.0563267505	2.2254349581	3.0242445342
C	0.4497812414	2.435052333	0.613558135
C	-0.741432591	3.1462391076	0.4589917042
C	-1.5292098115	3.3973102486	1.5901722909
C	-1.1454794804	2.9322056352	2.8503310101
C	0.6290528784	-0.1035392161	-0.6312253154
C	-1.7494245832	-3.3667958827	1.6934083755
C	-1.9353957047	-1.8926781388	1.9028574358
C	-2.3411720805	0.1387790094	0.6925013303
C	-3.7586020098	0.7581640713	0.5954319751
C	-4.0474208718	1.0073477152	-0.9083325609
C	-1.7784568047	0.4830281122	-0.6424021444
C	-0.8248646715	0.7293369406	-2.619814078
C	-2.1362996673	1.0890750126	-2.745265878

H	2.3414650571	3.4430337713	-1.5434613324
H	2.3350587925	1.8239361527	-2.2575925171
H	0.8434935298	2.7766192371	-2.186589163
H	0.3711173302	1.8694173885	3.9972201777
H	-1.0463488684	3.5090528946	-0.5164857059
H	-2.4523296622	3.9562117062	1.4852068818
H	-1.7765771154	3.1235747266	3.7102265449
H	-1.6523933873	-3.8685889181	2.6537579438
H	-2.577378492	-3.7861757301	1.1207304495
H	-0.8324741232	-3.5081980435	1.1140042843
H	-0.0275990258	0.6981715695	-3.3389514283
H	-2.6921589902	1.4384347582	-3.5974198199
H	-1.7598619545	0.5274675974	1.5235972741
H	-3.7610713539	1.7026357719	1.1373555725
H	-4.4938777213	0.0958747799	1.0482130681
H	-4.4758933883	1.9891879566	-1.1018962065
H	-4.6787037114	0.2420375379	-1.3598624043
C	2.0861067683	-1.7575369434	-1.5090005273
C	1.3006615872	-2.8963459826	-1.6665747684
C	3.453184354	-1.8425027436	-1.2837964084
C	1.9057181781	-4.1501077309	-1.5986923222
C	4.0508137946	-3.1023528081	-1.2278332158
C	3.281278006	-4.2558075342	-1.3830974075
H	0.2353346209	-2.7960533858	-1.8359803336
H	4.0153311203	-0.9303942475	-1.1314376738
H	1.3026903853	-5.0430583088	-1.7178961048
H	5.1178015421	-3.1800490797	-1.0526611926
H	3.7490388621	-5.2322934479	-1.3332038669
H	3.7490388621	-5.2322934479	-1.3332038669

TS 6-311++G(d,p) 0020

E(RB3LYP) = -1489.11988840 A.U.

First frequency = -219.9317 cm^{-1}

O	-1.2391633387	1.3921067088	2.6747891837
O	-0.3617675221	2.8756446559	1.1927329726
O	1.4900507534	-0.6885782238	-0.2641488589
O	-0.313186841	-1.3168391423	1.0353065334

O	-2.3633181367	-2.0242075078	-1.4287060154
O	-3.1176781489	-1.4212286084	0.6091905921
N	-0.5404186899	0.3468322955	-0.5616249251
N	-2.2532730481	1.2890824248	-1.4818843495
C	1.6160472624	0.1387353682	2.7526292374
C	-0.2690778048	1.7110060299	2.0059752499
C	1.0050035565	1.0880117932	1.7651202569
C	0.8660485376	3.0602135858	0.5957367265
C	1.2076145054	4.107780028	-0.2365164546
C	1.746664021	2.0208868217	0.9407469989
C	3.0423317452	2.0417959593	0.4199456716
C	3.4112724734	3.0881167821	-0.431586093
C	2.5086636357	4.107011953	-0.7590066254
C	0.2583470207	-0.494340705	0.3461069271
C	-2.6703836965	-3.7058371777	0.2783697873
C	-2.6991769446	-2.3259146829	-0.3042226375
C	-3.0465129082	-0.0238621248	0.2988784128
C	-4.2455793462	0.4601886336	-0.5658669525
C	-3.6993109194	1.5561026191	-1.5089468123
C	-1.8791658965	0.4462032741	-0.5241308468
C	-0.0717595414	1.1439748169	-1.6033988402
C	-1.1519310412	1.7433233321	-2.1766724764
H	2.051022251	0.6716169346	3.6058662249
H	0.8626081396	-0.5553902968	3.1281407015
H	2.4107261241	-0.4467162783	2.2839211411
H	0.4951331811	4.8868762183	-0.478979593
H	3.7472828135	1.2569743871	0.6667108763
H	4.4137805747	3.1125961983	-0.8443088284
H	2.8171961166	4.9084602252	-1.4203299385
H	-2.6256570851	-4.4429986467	-0.5205774591
H	-1.7688962629	-3.7802462331	0.8929396046
H	-3.5342200371	-3.8799297014	0.9199063691
H	0.9774708804	1.206566297	-1.824200524
H	-1.2223451153	2.4413385828	-2.9916674521
H	-3.0057380614	0.4589824039	1.2742829586
H	-5.059647712	0.8262180611	0.0557628453
H	-4.60486883	-0.3866352154	-1.1495545397
H	-3.8765990362	2.5638458962	-1.1323974283

H	-4.0745408124	1.4786577993	-2.5277376188
C	1.974273109	-1.9915041675	-0.3610852785
C	1.1888823838	-3.0203275463	-0.8786670542
C	3.2984528885	-2.2058948236	0.0033202722
C	1.7476991155	-4.2892961343	-1.0166415864
C	3.8495859471	-3.4781619586	-0.1498588713
C	3.0756751231	-4.5234234029	-0.6538755357
H	0.1629244057	-2.8288688841	-1.1663419414
H	3.881448846	-1.38234911	0.3959844976
H	1.1424835151	-5.0956586798	-1.41507794
H	4.8825118391	-3.6499606922	0.1302085593
H	3.5037222876	-5.5126630947	-0.7660800661
H	3.5037222876	-5.5126630947	-0.7660800661

TS 6-311++G(d,p) 0026

E(RB3LYP) = -1489.11999329 A.U.

First frequency = -203.3763 cm⁻¹

O	3.5547584106	0.6838697796	0.9045526985
O	1.8349588676	1.2244700092	2.2850466059
O	1.5611601407	-0.5853847019	-1.3557435118
O	0.401415195	-0.7799596154	0.6353567638
O	-2.3790228585	-2.0832253316	-0.718045478
O	-2.315000016	-1.0518255042	1.2866246778
N	-0.5345837184	0.3660567412	-1.1359923579
N	-2.5459909508	1.0753383241	-1.5001429752
C	2.0884637831	2.348196726	-1.2332231745
C	2.45683912	1.1912786822	1.0178773488
C	1.5484993976	1.7706501392	0.0455578354
C	0.6693612673	1.9459006126	2.1576053412
C	-0.2067977007	2.2538528194	3.1781143183
C	0.4922702461	2.3782784938	0.8319015048
C	-0.6075004595	3.1806365388	0.5238426793
C	-1.5052167799	3.5179637821	1.5453760163
C	-1.3156016632	3.0526522965	2.849909672
C	0.6346627168	-0.1745081617	-0.3993183118
C	-1.814631668	-3.3492778195	1.2603909856
C	-2.2083645687	-2.1323806487	0.4805655783

C	-2.4659883568	0.2496543979	0.7029966429
C	-3.9409718972	0.5632729019	0.3149201596
C	-3.9017907227	1.3594078429	-1.0106169264
C	-1.7522664605	0.5092543251	-0.5927337099
C	-0.5821349039	0.8452719192	-2.4410024777
C	-1.8462474259	1.3024987107	-2.6657681305
H	2.6749980552	1.6068951309	-1.7773136771
H	1.2795940821	2.6926054296	-1.8809721871
H	2.7327993709	3.2122171219	-1.0335918259
H	-0.0404134262	1.899220149	4.1877589107
H	-0.7621482355	3.5409864108	-0.4873299317
H	-2.3628947206	4.1415694931	1.3197809903
H	-2.0261036451	3.3166528528	3.6244362855
H	-0.7363522348	-3.2850824415	1.4317653679
H	-2.3127795435	-3.3753863221	2.2294843021
H	-2.0365116986	-4.2456017448	0.684900502
H	0.2777498372	0.795008855	-3.0822431367
H	-2.2919541103	1.7484907035	-3.5372876425
H	-2.0917157099	0.9221587888	1.4725679704
H	-4.4453626917	1.1165121486	1.1042700412
H	-4.4600694683	-0.3826876109	0.1665024494
H	-4.0017029748	2.4346263243	-0.857906054
H	-4.6399085678	1.0269091638	-1.7384012883
C	2.0430847166	-1.8911437189	-1.2318011313
C	1.1829249341	-2.9715722007	-1.4122576822
C	3.3966604189	-2.0716571415	-0.9815016004
C	1.7009911988	-4.2637627999	-1.3465234461
C	3.9067075516	-3.3695876876	-0.9297848123
C	3.06263109	-4.4658828998	-1.1109554051
H	0.128082126	-2.7976930459	-1.58919368
H	4.0168001157	-1.2017595672	-0.8068613764
H	1.0397930373	-5.1122243516	-1.4819131353
H	4.9625260356	-3.5219384899	-0.7366929484
H	3.4615568245	-5.4726264997	-1.0637521442
H	3.4615568245	-5.4726264997	-1.0637521442

TS 6-311++G(d,p) 0027
E(RB3LYP) = -1489.11826628 A.U.

First frequency = $-188.6931 \text{ cm}^{-1}$

O	1.0897205374	0.4581624391	-2.7237112619
O	2.6067031827	1.4764661753	-1.3788803325
O	0.1197219202	-0.9833839995	-0.2707122874
O	1.5025352055	0.1294505121	1.2172703956
O	-2.0684146911	-3.0594314377	-1.3679276818
O	-2.6010475196	-0.8779139789	-1.083123932
N	-0.798451524	0.4103593707	1.3213937504
N	-2.837215147	0.5502404074	2.0367796917
C	-1.0458547267	2.0401119328	-1.1752236543
C	1.2843542145	1.1611284436	-1.7511272222
C	0.3795303236	1.7611671134	-0.7867459494
C	2.5377654317	2.4265957654	-0.3800262635
C	3.617335078	3.0677687666	0.1940094786
C	1.2043329569	2.7047684209	-0.0464023389
C	0.9392692442	3.700903494	0.8922327286
C	2.0146389859	4.3694402686	1.4888376033
C	3.3343808035	4.0513817773	1.1525043809
C	0.4620554828	0.0746652776	0.579833553
C	-1.7433890954	-1.4914941841	-3.1816750714
C	-2.141715846	-1.9395183993	-1.8106687751
C	-2.7940301375	-1.0544503278	0.3193347485
C	-4.2653292126	-0.7526491657	0.7129975937
C	-4.2168421206	0.0348529176	2.0412111692
C	-2.0508578478	-0.0301006004	1.1269435868
C	-0.8103166792	1.2976987838	2.3874273358
C	-2.0927991344	1.3811758474	2.845146365
H	-1.5264125477	1.1507452304	-1.5790226093
H	-1.6268943512	2.381530046	-0.3142301468
H	-1.0984398596	2.8300489922	-1.9331287549
H	4.6334443745	2.8234618061	-0.0903746163
H	-0.081159962	3.956066699	1.1544991004
H	1.8226358635	5.147440539	2.2192167587
H	4.1528328025	4.5791154039	1.6285452305
H	-0.8365067089	-0.885743115	-3.0860037797
H	-1.5507021105	-2.3570624119	-3.8117038069
H	-2.5211397613	-0.8637366474	-3.6198512702

H	0.0972675959	1.7744664756	2.7091021457
H	-2.520611402	1.9456186256	3.6547562604
H	-2.4775981594	-2.0592501921	0.6025221821
H	-4.8545645516	-1.6631384539	0.7981517359
H	-4.6937839916	-0.1315645676	-0.07436999
H	-4.3476145139	-0.6039557192	2.9150761248
H	-4.9267043941	0.8586368775	2.0858117572
C	0.9385175997	-2.1152582719	-0.2498703065
C	0.9845694496	-2.923613648	0.8827128316
C	1.6254687598	-2.4518479615	-1.4084952138
C	1.7376806318	-4.0953470109	0.8487329342
C	2.3690140374	-3.6324503987	-1.4355878443
C	2.4295376799	-4.4540595189	-0.3100760252
H	0.4357053742	-2.6377204956	1.7714603455
H	1.5707734683	-1.7873389996	-2.260572623
H	1.779210514	-4.7304834977	1.7263612703
H	2.9054498769	-3.9050567059	-2.337418686
H	3.011179667	-5.3684013059	-0.3338200996
H	3.011179667	-5.3684013059	-0.3338200996

TS 6-311++G(d,p) 0028

E(RB3LYP) = -1489.11723524 A.U.

First frequency = -205.6093 cm^{-1}

O	1.2890522074	0.4223694618	-2.5614326867
O	2.7333028492	1.4027320592	-1.1128044102
O	0.1235920727	-1.0303198208	-0.1819602838
O	1.3382681605	0.1056533091	1.4344838941
O	-2.3446750381	-2.969622941	-1.7503757565
O	-2.4847012254	-0.7471166437	-1.3673593134
N	-0.9575261456	0.3926283211	1.2662110475
N	-3.0611158595	0.6006169395	1.7381792832
C	-0.8953294511	2.0902120521	-1.1774802587
C	1.4303795956	1.1184968049	-1.5786673043
C	0.4732415788	1.7274428456	-0.6656137147
C	2.6166026305	2.3441975531	-0.1080096706
C	3.6692324359	2.9550134489	0.5436413348
C	1.2713554555	2.6447861699	0.1411106554

C	0.9640369628	3.6311606825	1.0756478644
C	2.0106570253	4.2701028854	1.7512216363
C	3.3429396666	3.9308749077	1.4962594242
C	0.3857687434	0.0567055866	0.6690231416
C	-1.5380185144	-1.4039367715	-3.4119269316
C	-2.158067845	-1.8351977026	-2.1201858778
C	-2.8767117173	-0.9550161351	-0.0112435873
C	-4.3704628101	-0.5887487614	0.2040218331
C	-4.4521630724	0.1543767671	1.5556173442
C	-2.193019438	0.007176773	0.9144086972
C	-1.0652040146	1.259518539	2.3434826074
C	-2.3889710912	1.384678302	2.6488685128
H	-1.541694984	2.4297552294	-0.3637811895
H	-0.8330761534	2.9101699888	-1.9017981697
H	-1.3730326627	1.2427249679	-1.6641552991
H	4.6967752536	2.6943266904	0.3218765937
H	-0.0663585418	3.9020570631	1.2757203606
H	1.7860905933	5.0407246206	2.4800568809
H	4.1385254045	4.4355288574	2.0322774703
H	-0.576918947	-0.9308565651	-3.187427708
H	-1.3960043132	-2.2662218592	-4.0593916391
H	-2.1667372477	-0.658198853	-3.9022691794
H	-0.1857891017	1.6949389763	2.7814365689
H	-2.8893713411	1.9489173043	3.4158869175
H	-2.6534952372	-1.9825720029	0.2768889256
H	-5.0089846256	-1.4692786895	0.1803847192
H	-4.6637568223	0.0781370017	-0.6075605471
H	-4.7196098699	-0.5037013073	2.3828606118
H	-5.1237723868	1.0105973657	1.5428382085
C	1.0246403723	-2.0929531338	-0.2152950205
C	0.4708737064	-3.3682385414	-0.1325855289
C	2.3968384966	-1.9187020141	-0.3879292983
C	1.2990663683	-4.4859071761	-0.2274217927
C	3.2152955492	-3.0444893654	-0.4697095416
C	2.6748965209	-4.3288767893	-0.3925591855
H	-0.5988930006	-3.475454529	-0.0151609854
H	2.8161575753	-0.9265815342	-0.4525691707
H	0.864857608	-5.4776431249	-0.1691158909

H	4.2833746715	-2.911936805	-0.6013355184
H	3.3195573998	-5.1974027982	-0.4628078046
H	3.3195573998	-5.1974027982	-0.4628078046

TS 6-311++G(d,p) 0030

E(RB3LYP) = -1489.12098490 A.U.

First frequency = -247.4722 cm⁻¹

O	-0.8182806676	1.4349857396	2.6453577491
O	-0.1927143847	2.8395251545	0.9793266075
O	1.166327674	-0.8367696806	-0.7527385452
O	-0.2418018283	-1.3621093461	1.029257874
O	-3.8491812441	-1.4804629622	-1.385756208
O	-3.2703659488	-1.589649165	0.7912439118
N	-0.813100568	0.2343915046	-0.5541269588
N	-2.6817125253	1.2383426485	-0.9827612825
C	1.9770761928	0.1476040548	2.2859817182
C	0.0050143051	1.6938632655	1.787774154
C	1.1843958434	0.9887667823	1.3194321624
C	0.9083214394	2.9594350594	0.1558609075
C	1.1278573166	3.9832116756	-0.7448055923
C	1.7958661662	1.8911248103	0.3516239944
C	2.9762419228	1.8578407008	-0.3907439397
C	3.2230646011	2.8791822276	-1.3134917401
C	2.311243698	3.9258574643	-1.4932461177
C	0.1886266088	-0.5685004493	0.205903773
C	-3.8252603717	-3.6185486569	-0.254588429
C	-3.6677474309	-2.1305692041	-0.3799009281
C	-3.0079586198	-0.1680252089	0.8836756829
C	-4.2581119889	0.7349660769	0.677202437
C	-4.1119233232	1.4247707037	-0.7011386128
C	-2.0897579609	0.3687987401	-0.1678886794
C	-0.6121746695	1.0361195677	-1.6715722426
C	-1.7939261038	1.6640355364	-1.9431067377
H	2.8032276307	-0.3529950519	1.7784433814
H	2.3977203027	0.7628220144	3.0890839799
H	1.3428379248	-0.6180926787	2.7348215436
H	0.4126127918	4.7874033058	-0.8661767894

H	3.6862521038	1.0506959304	-0.2588747798
H	4.1358443961	2.8615218534	-1.8984690683
H	2.5223397955	4.7064446916	-2.2149764426
H	-2.8423854104	-4.0659501192	-0.0866194268
H	-4.4506477463	-3.861273311	0.6060333407
H	-4.2613281942	-4.0191881055	-1.1669256153
H	0.3482367095	1.0951422217	-2.148301229
H	-2.0552011768	2.3716722859	-2.7097699858
H	-2.5712243012	-0.0608360216	1.8706667508
H	-4.2721653901	1.4839133268	1.4687046432
H	-5.1723148132	0.1485287566	0.7454459084
H	-4.3477137629	2.4871326155	-0.6742157995
H	-4.6863777832	0.9314033053	-1.4832784112
C	2.1964584947	-1.7445597264	-0.5731748658
C	3.2952900491	-1.5332703433	-1.4089730612
C	2.1709648435	-2.827948134	0.3074139302
C	4.3812319438	-2.4017440643	-1.358675955
C	3.2725939232	-3.6839179473	0.3514287075
C	4.3783029716	-3.4806909095	-0.4728181693
H	3.2826297289	-0.6863116285	-2.0834210095
H	1.3183928375	-2.9870448685	0.9476040644
H	5.2312524705	-2.2307134177	-2.0094265561
H	3.256828923	-4.5216042041	1.0397526926
H	5.2257445872	-4.1546098474	-0.428094535
H	5.2257445872	-4.1546098474	-0.428094535

TS 6-311++G(d,p) 0036

E(RB3LYP) = -1489.12094498 A.U.

First frequency = -208.9059 cm^{-1}

O	3.5315836816	0.4596315515	1.830239935
O	1.599475388	1.3182697145	2.6530659316
O	2.0022330112	-0.9241017685	-0.6966242064
O	0.3220576744	-0.6925678903	0.8806869101
O	-2.8682994846	-1.4654708823	-1.6308676765
O	-2.6096758252	-0.6906921934	0.4699123904
N	0.086536118	0.2667866891	-1.2056795717
N	-1.6170603494	1.1705333748	-2.1923972436

C	2.8489832016	1.9524389136	-0.7743224893
C	2.5060130799	1.0703534645	1.6012729293
C	1.9437011815	1.6025923415	0.3736775851
C	0.6007816898	2.126606376	2.1587714161
C	-0.4559461168	2.6394421243	2.8826125052
C	0.8125916263	2.4056204905	0.7975120111
C	-0.0666871393	3.2678990248	0.1408290312
C	-1.1384981198	3.8148755241	0.8581646926
C	-1.3397399826	3.4954341985	2.2035540419
C	0.9197075782	-0.2796560728	-0.100063634
C	-3.1093171487	-2.9757738028	0.2422106538
C	-2.8672311455	-1.6583342234	-0.4344139863
C	-2.2382528593	0.6324066192	0.0197987533
C	-3.3879647362	1.4194506358	-0.6722343595
C	-3.0421507918	1.526034822	-2.177860835
C	-1.1835217791	0.6621731489	-1.0405163717
C	0.4528955691	0.5305012552	-2.5205461667
C	-0.6228623105	1.0968886737	-3.141182566
H	3.4592637285	1.0952651507	-1.0617797475
H	2.2738725756	2.2746867664	-1.6449092351
H	3.5222434298	2.7755373216	-0.508474991
H	-0.5908580622	2.3962766465	3.9292610238
H	0.0803291339	3.5166836464	-0.9044515713
H	-1.8246984004	4.4913076427	0.3612233907
H	-2.1820492992	3.9193225	2.7376106994
H	-3.7665007599	-2.8527482663	1.103626507
H	-3.5343531235	-3.6809602653	-0.46876817
H	-2.1507847272	-3.356832764	0.6053713147
H	1.4322114906	0.2824487285	-2.8848967587
H	-0.7522580119	1.4409259348	-4.1522288621
H	-1.8998100246	1.1147401244	0.9318329013
H	-3.4384573715	2.4117919345	-0.2266738913
H	-4.3414167313	0.9207929365	-0.5096417412
H	-3.1789995124	2.5295828281	-2.5773686874
H	-3.5836448466	0.8036666191	-2.7870341662
C	2.2015634433	-2.2615719376	-0.3328280956
C	1.4406801833	-3.2506955126	-0.9494403252
C	3.1886960138	-2.5732447022	0.5923763699

C	1.6805477767	-4.5867978639	-0.6312562193
C	3.425322934	-3.913949614	0.8990880756
C	2.6742164413	-4.9206155151	0.2908808501
H	0.6762367484	-2.9714714178	-1.6648340699
H	3.7378223378	-1.7673482583	1.0625403063
H	1.0936859132	-5.3648183343	-1.1061269246
H	4.1942545639	-4.1696698738	1.6192497309
H	2.860427683	-5.9601854938	0.5348649138
H	2.860427683	-5.9601854938	0.5348649138

TS 6-311++G(d,p) 0040

E(RB3LYP) = -1489.12159424 A.U.

First frequency = -203.9497 cm^{-1}

O	3.3555493604	0.2727741012	1.8375638534
O	1.3520454707	1.0096350748	2.6092434622
O	2.0100401472	-0.8752533258	-0.8754803706
O	0.1965458766	-0.7713620525	0.560441373
O	-2.9428297524	-0.8275887739	1.8221977806
O	-2.609256008	-0.8090580945	-0.4151542488
N	0.1520798495	0.3747511706	-1.4420699727
N	-1.4862680056	1.3347611116	-2.487958907
C	2.8219416893	2.0255584225	-0.6382978122
C	2.3369403406	0.8949986749	1.6060211643
C	1.8536709424	1.5587259471	0.4110312504
C	0.3752928854	1.8575387719	2.1374745209
C	-0.7412805628	2.2710437186	2.8332753684
C	0.6809307029	2.2950289571	0.8365573165
C	-0.1649915159	3.2176157314	0.2185644826
C	-1.2963305529	3.6664357302	0.9127056298
C	-1.5891102865	3.1905253817	2.1930805691
C	0.8791023082	-0.2813862158	-0.3250194655
C	-2.8508894832	-2.91405312	0.6046541074
C	-2.818092109	-1.4243023144	0.780841651
C	-2.2616184037	0.5928704375	-0.3929574504
C	-3.3498744478	1.4719837292	-1.0600724456
C	-2.9110516212	1.7075811228	-2.5293503589
C	-1.1256802826	0.7625517271	-1.3405644086

C	0.6115796372	0.7320716051	-2.7048058129
C	-0.421445367	1.3350017717	-3.3638581785
H	2.2961950737	2.4303225028	-1.5059277983
H	3.4704039174	2.8208080374	-0.2527936958
H	3.4575954284	1.2040655651	-0.9722121047
H	-0.95041228	1.9030069238	3.8299379064
H	0.0552502562	3.5902704324	-0.7758120902
H	-1.9567243858	4.3896309716	0.4475096011
H	-2.4774711906	3.5384997778	2.7069438404
H	-1.8209630713	-3.2564642612	0.4685989942
H	-3.274849287	-3.3830488847	1.4899692189
H	-3.4171447285	-3.1883808719	-0.2861019855
H	1.6172335251	0.5147441273	-3.0133397824
H	-0.4782898781	1.7488146834	-4.3551833547
H	-2.0296635897	0.8963835661	0.6238022575
H	-3.400976725	2.4212850535	-0.5291053356
H	-4.3214805595	0.9858998275	-0.9970363045
H	-3.0147765608	2.7449037731	-2.8428321573
H	-3.4232466842	1.0615328902	-3.2423523823
C	2.2190359266	-2.2242510196	-0.5676275413
C	3.3116465479	-2.5645520772	0.2180093306
C	1.3722462869	-3.193601923	-1.0986091433
C	3.5695768895	-3.9131875593	0.4673469995
C	1.6327957066	-4.5372070372	-0.8350584802
C	2.7329861642	-4.8998977862	-0.0554060896
H	3.919582531	-1.7739605691	0.6381809622
H	0.5248165405	-2.8947455332	-1.7037791927
H	4.420389784	-4.1899714595	1.0794684873
H	0.978290137	-5.2996088503	-1.2419719086
H	2.9341200454	-5.9458063219	0.1456778583
H	2.9341200454	-5.9458063219	0.1456778583

4.2 Minor enantiomer

4.2.1 Starting TS

TS input

E(RB3LYP) = -1488.74935124 A.U.

First frequency = $-208.0832 \text{ cm}^{-1}$

O	-1.4087617543	-2.7481900184	0.6640895067
O	0.2295635904	-2.8290224215	-0.9116082011
O	1.1100108414	0.8604443288	1.2334432264
O	0.2782869624	0.1847301131	-0.8371978995
O	-3.5366003665	2.0591315123	-0.7931050869
O	-2.4822309068	0.4585366917	-1.9995234216
N	-1.0952443765	0.2404119022	1.0266823018
N	-3.2316413203	-0.046643262	1.2625132711
C	0.8121330187	-1.7825275585	2.5987937037
C	-0.2407347126	-2.5132499791	0.3760562352
C	0.8029851751	-1.809343684	1.0954104234
C	1.5753160019	-2.5150114918	-0.9461884805
C	2.4256257544	-2.7389252814	-2.0138679571
C	1.9962708733	-1.9695581666	0.2779693588
C	3.340969069	-1.6393354734	0.4451496741
C	4.2254003988	-1.859681398	-0.6190330032
C	3.7743546331	-2.3939096511	-1.8323886241
C	0.2469571783	0.1472432012	0.3885744084
C	-2.5443118359	2.6116749529	-2.9343282884
C	-2.9291393655	1.7161165445	-1.7885287984
C	-2.6492069325	-0.5447518569	-0.9739794247
C	-4.1227919779	-0.9630167083	-0.6997756143
C	-4.5366428318	-0.3449541735	0.6599214846
C	-2.2210998666	-0.1216911925	0.3971631525
C	-1.4209651979	0.5619801806	2.3397317053
C	-2.7690742873	0.3850010209	2.4851792126
H	1.3517886099	-0.9068791646	2.9701368858
H	-0.2085386714	-1.7548337035	2.9882187578
H	1.3003610758	-2.6754370601	3.0082836057
H	2.0624496783	-3.1647293023	-2.943005985
H	3.6909226301	-1.2101874411	1.3789032194
H	5.2751591959	-1.6064533647	-0.5038348654
H	4.4761868822	-2.5511993898	-2.6457893464
H	-1.4551845207	2.7166516338	-2.9498409177
H	-2.8464146306	2.1641616051	-3.8843134159
H	-3.0090578724	3.5885057303	-2.8081138559

H	-0.6671352494	0.8846949564	3.0354258104
H	-3.4122451864	0.5292253937	3.3373850098
H	-2.0449877581	-1.3708894073	-1.3369493319
H	-4.1539420833	-2.0519814562	-0.6332736106
H	-4.7745115797	-0.6449428686	-1.513520327
H	-5.090692241	-1.037486629	1.2942577869
H	-5.088696872	0.588841414	0.5479706734
C	1.9503892587	1.8293619515	0.6939371974
C	2.761813686	1.6025946623	-0.4199610243
C	1.9969724634	3.0411226706	1.3846937706
C	3.6197889323	2.6193805853	-0.8433306894
C	2.8694799285	4.0432002638	0.9572579719
C	3.6809182335	3.8373786864	-0.1610355391
H	2.7169814646	0.6523704004	-0.9317227816
H	1.35217181	3.1812392945	2.2460963111
H	4.2515950956	2.4499719622	-1.7104081768
H	2.9089625754	4.9846769701	1.4970182882
H	4.3570463804	4.6178724754	-0.4962482859
H	4.3570463804	4.6178724754	-0.4962482859

4.2.2 Lowest TS

TS 6-311++G(d,p) 0010

E(RB3LYP) = -1489.12202589 A.U.

First frequency = -264.0308 cm^{-1}

O	-1.7512198772	-1.9419845976	1.4530101417
O	-0.3011292497	-2.602523005	-0.150808133
O	0.9550945628	1.5292252941	0.9938665567
O	0.0678347022	0.3718196733	-0.8313367879
O	-2.3119168997	-0.7370151398	-3.3264619275
O	-2.8287559379	0.8734821867	-1.8264937701
N	-1.2370465741	0.9626291849	0.9974000542
N	-3.3856257284	0.9395854224	1.2874420726
C	0.7181778472	-0.7759563251	2.8895072678
C	-0.6135241914	-1.8998860962	1.0175645608
C	0.5506094017	-1.1275264046	1.4346431795
C	1.0601216822	-2.4719741858	-0.3624218375

C	1.7739612811	-3.0981022393	-1.3655203657
C	1.6431194397	-1.6564574157	0.6140579426
C	3.0251556092	-1.4813453788	0.6040227942
C	3.7766124276	-2.1084028961	-0.3940347864
C	3.1603296665	-2.8966630718	-1.3719824747
C	0.0807328167	0.6162470023	0.3703794125
C	-2.2717370221	1.5852557672	-3.9975141174
C	-2.4637894801	0.4305524334	-3.0570535772
C	-2.8952830971	-0.1021736079	-0.76015259
C	-4.3572416763	-0.415767804	-0.3573014771
C	-4.7198822314	0.5652260803	0.7862827889
C	-2.400841461	0.5698513474	0.4725100075
C	-1.5069896105	1.5992107409	2.2037459055
C	-2.8607361095	1.5889092885	2.383726114
H	1.1185377081	-1.6260290472	3.4523995983
H	1.404768429	0.0621545551	3.0125227381
H	-0.2397850646	-0.5046052109	3.3357617248
H	1.2816021811	-3.718535324	-2.1040408816
H	3.5085690167	-0.8536545343	1.3422311868
H	4.8521267449	-1.9743602541	-0.4156555604
H	3.7611899618	-3.3663632534	-2.1423079198
H	-2.1982195254	1.2193429056	-5.0193050563
H	-3.0915556373	2.2985262685	-3.9031664293
H	-1.3465173648	2.101248954	-3.7272076762
H	-0.7178613919	2.0033364165	2.809633968
H	-3.4688676073	1.9803964882	3.1799941838
H	-2.321542516	-0.9812279224	-1.033487317
H	-4.3960951352	-1.4403995478	0.012025393
H	-5.025416186	-0.3236635204	-1.211401144
H	-5.2989564271	0.0987631929	1.5808415189
H	-5.2347708774	1.4615466107	0.4393905899
C	2.2561209786	1.7200449208	0.5600461494
C	2.6389535666	1.735416985	-0.7823326836
C	3.1864287252	1.9758593425	1.5684088326
C	3.9760527659	1.9729867272	-1.0978685387
C	4.5160803911	2.2219063699	1.2370242182
C	4.9197001952	2.2121620432	-0.0988598073
H	1.9102597159	1.5405154757	-1.552977093

H	2.8587916628	1.9708507444	2.6008432414
H	4.2786397674	1.9714086862	-2.1390922141
H	5.2360379288	2.4146276071	2.0243346515
H	5.9560076602	2.3948292541	-0.3581916356
H	5.9560076602	2.3948292541	-0.3581916356

4.2.3 Additional TS

TS 6-31G(d,p) 0001

E(RB3LYP) = -1488.74902322 A.U.

First frequency = -212.5221 cm^{-1}

O	-1.7225238811	-1.970643596	1.5875622405
O	-0.274953695	-2.7247439051	0.0087181566
O	0.8505425679	1.5159199787	0.7784453667
O	0.051330258	0.1517185024	-0.9462197081
O	-2.5724965253	2.0051534435	-1.8658764111
O	-2.4681042014	-0.2391519489	-2.1339184306
N	-1.3119916571	0.8474251291	0.8044688264
N	-3.45728613	0.8040864223	1.1009182506
C	0.725510885	-0.6202387388	2.8801470394
C	-0.5861976593	-1.9430127093	1.131898769
C	0.5651634285	-1.1182191671	1.4683432897
C	1.0786912885	-2.5760661023	-0.2331876383
C	1.7941909811	-3.2558629749	-1.2030109993
C	1.6595509179	-1.6783884988	0.6760586373
C	3.0372353911	-1.4648966515	0.621303175
C	3.7876205516	-2.1421858264	-0.3469599034
C	3.1755921433	-3.0181720601	-1.2525794662
C	0.0234502222	0.5172133308	0.2285649091
C	-1.4666227939	1.0698709858	-3.8100307509
C	-2.2290503844	1.0394316313	-2.5177752054
C	-2.9839365664	-0.4650309974	-0.8221790912
C	-4.5163016673	-0.2129368244	-0.719591721
C	-4.7782994285	0.2875932362	0.7186539924
C	-2.4713635625	0.4078877638	0.2946209575
C	-1.5924141662	1.5496868291	1.9735329556
C	-2.9425780172	1.5133012939	2.1654253875

H	-0.2505079887	-0.3869841887	3.3128677033
H	1.1992985711	-1.3778820494	3.5161953693
H	1.343103973	0.2797508608	2.9157839371
H	1.3042600255	-3.9429378239	-1.8845213478
H	3.515144629	-0.768577594	1.3020283078
H	4.8598617781	-1.9787261511	-0.401678681
H	3.7759810219	-3.5274891425	-2.0004092023
H	-0.43313565	0.7916391096	-3.5813374437
H	-1.8657035069	0.3400695456	-4.5174967388
H	-1.4938897973	2.0733108838	-4.2331218672
H	-0.8082191074	2.0213942459	2.5377429559
H	-3.5607013191	1.9352138136	2.9402982266
H	-2.7198964078	-1.4994755133	-0.6000472309
H	-5.0874962189	-1.1113438947	-0.9518069883
H	-4.7762332113	0.5676081307	-1.4359822048
H	-5.0508692719	-0.519771436	1.4026800665
H	-5.5265639748	1.078673722	0.7766865151
C	2.1468736284	1.7091294681	0.3320363448
C	3.0750449402	2.0515729415	1.3195546424
C	2.5244778452	1.6526047549	-1.0134560748
C	4.3995269102	2.3059932719	0.9658822726
C	3.8565433662	1.8985951561	-1.3497219495
C	4.7993203666	2.2195833791	-0.3702332016
H	2.747998577	2.1107020138	2.352149685
H	1.7922765391	1.3977203856	-1.7650735288
H	5.1183251669	2.5666652655	1.7369658193
H	4.1556554772	1.841418215	-2.3922878077
H	5.8321483761	2.4088068031	-0.6456777469
H	5.8321483761	2.4088068031	-0.6456777469

TS 6-31G(d,p) 0010

E(RB3LYP) = -1488.75073277 A.U.

First frequency = -219.6892 cm^{-1}

O	-1.7921085284	-1.9092919975	1.4546641296
O	-0.3689892438	-2.5423925756	-0.1978032615
O	0.9235674989	1.5499174635	0.9970930956
O	0.0196276502	0.4181049042	-0.8422976611

O	-2.0234365413	-0.8540197017	-3.1634387835
O	-2.8407320461	0.7776286408	-1.8108674163
N	-1.2648780471	0.9820893296	1.007359231
N	-3.4119066312	0.9438496527	1.3175851333
C	0.6977746049	-0.7719938443	2.8717011551
C	-0.6541151606	-1.8733161628	1.0022058707
C	0.52295443	-1.1266786842	1.4195426369
C	0.9881006376	-2.4112077357	-0.4292166101
C	1.6802736671	-3.0075493121	-1.4682730554
C	1.5983520427	-1.6356422139	0.5689369469
C	2.9831850518	-1.4678217626	0.5353562346
C	3.7104481165	-2.064617519	-0.500682272
C	3.0691643403	-2.8152526166	-1.4944845867
C	0.0418464371	0.6566482281	0.3652558967
C	-1.944885595	1.4594900144	-3.8764122488
C	-2.2578939206	0.3150935932	-2.9531845622
C	-2.9237969459	-0.1509818085	-0.7108775377
C	-4.3882139504	-0.444197022	-0.2977304478
C	-4.7466960862	0.5608095479	0.8281662688
C	-2.4288454502	0.5579186292	0.5040425293
C	-1.5299397934	1.6430657929	2.2023457989
C	-2.884049433	1.6234855036	2.394688116
H	1.1027906743	-1.616810196	3.4419396399
H	1.3808690633	0.0717002867	2.9916824412
H	-0.2641192513	-0.5029574518	3.3158261954
H	1.1665036049	-3.5982567391	-2.2188903124
H	3.4847006034	-0.8667276281	1.2862251795
H	4.7879988845	-1.9351183622	-0.5392440652
H	3.6525020553	-3.2619300607	-2.2940274219
H	-1.7095650539	1.0801840353	-4.8700507261
H	-2.7770511355	2.165425576	-3.9194813238
H	-1.0761978086	1.9885921892	-3.4710630279
H	-0.736575694	2.0701347623	2.7895729701
H	-3.4910900308	2.0307236193	3.1860845425
H	-2.3581424679	-1.0470855386	-0.9505178891
H	-4.4277105134	-1.4611096171	0.0968629024
H	-5.0586363853	-0.3677104776	-1.1537447846
H	-5.3265240095	0.1119011903	1.6348805084

H	-5.2627349648	1.4525460611	0.4650627167
C	2.222505215	1.7336442772	0.5527401255
C	2.5922038821	1.7630095318	-0.7955276063
C	3.1651771002	1.9682954234	1.5577958783
C	3.9309627334	1.9879878247	-1.120059425
C	4.4963255093	2.2026681827	1.2160315294
C	4.8876973043	2.203411587	-0.1253947626
H	1.8496949478	1.5854448329	-1.5593112612
H	2.8433594505	1.9590760742	2.5937747893
H	4.2244876315	1.9966952258	-2.1656967399
H	5.2266671991	2.3792483571	1.9999882596
H	5.9254043089	2.3771798773	-0.3924919403
H	5.9254043089	2.3771798773	-0.3924919403

TS 6-31G(d,p) 0012

E(RB3LYP) = -1488.75203680 A.U.

First frequency = -215.4867 cm^{-1}

O	1.97434915	-0.6220571046	2.9874082015
O	0.2799585153	-2.0515676243	2.4585023662
O	0.9550049827	1.4369692617	0.9975945706
O	0.7371657881	0.5945171355	-1.1603483299
O	-2.1031615201	2.144772819	-1.6087888496
O	-1.5289653299	0.3066734619	-2.7982694001
N	-0.8683092947	0.1973569155	0.4709033255
N	-2.934447552	-0.4366390568	0.3723361321
C	2.9027565656	-1.0333152446	0.0283854111
C	1.4039218219	-1.2454208787	2.1061551236
C	1.5682737386	-1.2962578104	0.6690306305
C	-0.1376690538	-2.6982617383	1.3176597159
C	-1.1994620898	-3.5811257007	1.2325629637
C	0.6570681923	-2.332667537	0.2140102997
C	0.3995404567	-2.9200232366	-1.0260695936
C	-0.659170912	-3.8351196326	-1.1338480374
C	-1.4567602261	-4.1501916731	-0.026969066
C	0.5086101427	0.5294563247	0.0437540987
C	-0.723060073	2.3706695778	-3.588189944
C	-1.536036653	1.6424742045	-2.558103393

C	-2.0650604614	-0.566065881	-1.805597564
C	-3.6158509091	-0.6670698257	-1.8481732058
C	-4.0602181107	-0.9790685236	-0.4022894546
C	-1.8408329215	-0.2127735334	-0.357367773
C	-1.388652357	0.254292834	1.7612468426
C	-2.6860807273	-0.1603946118	1.7010900352
H	2.7694697314	-0.5815698588	-0.9599556277
H	3.4949315138	-0.3480272527	0.6381585106
H	3.4724072819	-1.96255239	-0.0970065455
H	-1.7970932036	-3.8253149314	2.1041787205
H	1.0009992368	-2.6609187486	-1.8918553413
H	-0.8684475339	-4.3002945545	-2.0928443495
H	-2.2768468106	-4.8533611494	-0.1349671766
H	0.3306882774	2.2092631908	-3.339457348
H	-0.9020265592	1.9692555466	-4.5875705268
H	-0.9498379854	3.4356304057	-3.5525166116
H	-0.777261539	0.5666263096	2.5889753309
H	-3.4309911669	-0.2736262847	2.4707221476
H	-1.5914386885	-1.5275274977	-2.0074377826
H	-3.9506030767	-1.424803732	-2.5560715459
H	-4.007689796	0.3046473004	-2.1535343772
H	-4.1345796589	-2.0513195079	-0.205651847
H	-4.9904873518	-0.4896372595	-0.1134673653
C	2.0332062479	2.2595385664	0.6947269526
C	1.9788574429	3.1551934766	-0.3742601741
C	3.1272596818	2.2147905506	1.5570772674
C	3.0582252434	4.0145834827	-0.5849893604
C	4.1952519191	3.087011794	1.338909265
C	4.1659299402	3.9840289741	0.2675001675
H	1.1060832116	3.1701552899	-1.0149767008
H	3.1182127585	1.4887159044	2.3625766803
H	3.0289123417	4.7146220302	-1.4146901772
H	5.0527634929	3.0608079114	2.0046674576
H	5.0002085324	4.6579495338	0.098532025
H	5.0002085324	4.6579495338	0.098532025

TS 6-31G(d,p) 0015

E(RB3LYP) = -1488.74668956 A.U.

First frequency = $-224.8580 \text{ cm}^{-1}$

O	-1.7865735335	-1.9581590078	1.3920693086
O	-0.366454553	-2.5294500827	-0.2843410986
O	0.9210926293	1.5144870938	1.0456162609
O	0.0329118601	0.4342102654	-0.8293492738
O	-2.1113256858	1.5195051933	-3.7338584282
O	-2.9073237864	0.7813885807	-1.822729452
N	-1.2677879279	0.9443367054	1.0188772921
N	-3.4172503382	0.8907150981	1.3030192143
C	0.7034159166	-0.8612624033	2.8430249747
C	-0.6490599293	-1.9052840417	0.9417512748
C	0.5276865335	-1.1702354234	1.3806028947
C	0.992256895	-2.3907159059	-0.5123672521
C	1.6797453558	-2.9423815817	-1.57870088
C	1.6028369769	-1.6497134819	0.5108442518
C	2.9863908104	-1.4728435031	0.4752295567
C	3.7101695419	-2.0259492845	-0.5873392398
C	3.0674375562	-2.7417182741	-1.6054457323
C	0.0465592443	0.63715757	0.3869482155
C	-1.5770327956	-0.7713738601	-3.2301041647
C	-2.1839253227	0.5849096682	-2.9679973157
C	-2.9098179529	-0.1668925878	-0.7417760962
C	-4.3605690507	-0.5093849116	-0.3159692829
C	-4.7434647746	0.4929152155	0.8022331507
C	-2.4240797684	0.5273742103	0.4912982793
C	-1.5487963442	1.5778518143	2.2244834346
C	-2.9050846344	1.5489187502	2.4003131648
H	-0.2550310592	-0.5880223093	3.292056637
H	1.0918136462	-1.7292211718	3.3891677112
H	1.4003443185	-0.0332958841	2.9882677658
H	1.1648005585	-3.5081318703	-2.3476061342
H	3.4895433111	-0.897188895	1.2444722704
H	4.7866090106	-1.8887364714	-0.6274000105
H	3.648354414	-3.1538552043	-2.4249098983
H	-1.1544641235	-0.7557722897	-4.23374886
H	-0.7892651416	-0.9797114422	-2.5028147592
H	-2.3307561035	-1.5618872023	-3.1667634598

H	-0.7637557714	1.9959381927	2.8292518919
H	-3.5232222997	1.9369069952	3.1927784199
H	-2.3241090045	-1.0499748254	-0.9728754918
H	-4.359772175	-1.522582913	0.0900237202
H	-5.0373256268	-0.4635493077	-1.1691036278
H	-5.3254422801	0.0390558762	1.6044393461
H	-5.2655754569	1.3774632322	0.4308202259
C	2.216945662	1.7239627831	0.5998902459
C	3.1679823084	1.9127777391	1.6063063754
C	2.5723375283	1.8207459561	-0.7489051421
C	4.4951653268	2.1673065893	1.2632465958
C	3.9072108291	2.0656031415	-1.0752051502
C	4.8731148569	2.2341579475	-0.080348602
H	2.8563939087	1.8531903374	2.6436931639
H	1.8221545686	1.6815859821	-1.5132161071
H	5.2327814741	2.3081161662	2.047587259
H	4.1900234773	2.1278358433	-2.1219377624
H	5.9076648129	2.4240052742	-0.3487166251
H	5.9076648129	2.4240052742	-0.3487166251

TS 6-31G(d,p) 0016

E(RB3LYP) = -1488.74339982 A.U.

First frequency = -188.8248 cm^{-1}

O	1.4338434647	-2.1344248556	-2.3146495092
O	2.5407861992	-2.113691154	-0.3160737514
O	1.1432006703	0.4876347464	0.2403733241
O	-0.323253452	0.272206588	-1.5521235682
O	-2.3372874895	2.7361048808	-0.6193207619
O	-3.0008465951	1.0117898082	-1.9253543655
N	-1.0665454942	0.1571270175	0.6435976978
N	-3.0258467718	0.3398445651	1.5478915222
C	-1.1221683278	-2.6393951121	-0.6852151865
C	1.3541154577	-2.17280702	-1.0952204645
C	0.2239559498	-2.1916285409	-0.2005211862
C	2.1736087603	-2.2781126127	0.9991039639
C	3.0384432142	-2.3363194174	2.0753303877
C	0.7737343249	-2.4087581685	1.1200336017

C	0.2293969449	-2.6491262108	2.385439394
C	1.0885789102	-2.7177959502	3.491376857
C	2.4703207888	-2.5538873071	3.342859386
C	-0.0138360708	0.0648761936	-0.3875646473
C	-1.9026551353	2.7966702862	-3.0022245567
C	-2.4290383862	2.2277493344	-1.7184156879
C	-3.3395819085	0.228755791	-0.7818709497
C	-4.660263997	0.6840403389	-0.0932548306
C	-4.4889232137	0.3998170048	1.4167977418
C	-2.3823146882	0.2508568072	0.3829130127
C	-0.8902409094	0.2194663262	2.0241548647
C	-2.1265542744	0.3244041549	2.5928818256
H	-1.3728900815	-2.116374288	-1.6131601809
H	-1.1546445146	-3.7170563448	-0.8878539793
H	-1.8993284522	-2.4297509023	0.0578907795
H	4.1091831801	-2.2265011058	1.9393771981
H	-0.8418896952	-2.7752729248	2.5091919089
H	0.6747982901	-2.9019337388	4.4787546572
H	3.1173392039	-2.6069792659	4.213213693
H	-1.7583492479	3.8715837221	-2.8984679863
H	-0.937513258	2.3143349399	-3.1879259339
H	-2.5663340611	2.5707644185	-3.8385622895
H	0.0919289008	0.1857199474	2.4583532858
H	-2.4282044291	0.3891631811	3.6249247633
H	-3.4134443046	-0.7877530028	-1.1724568964
H	-5.5270394694	0.1734661589	-0.511729163
H	-4.7679517401	1.7568166576	-0.2567854928
H	-4.9118685404	-0.5607984967	1.719770836
H	-4.8901086037	1.1868869354	2.0559964534
C	2.0868156897	1.242580593	-0.4537393733
C	2.6298399904	2.3084201724	0.2642558114
C	2.5212586806	0.9384281569	-1.7443446329
C	3.6257719567	3.0912404208	-0.3202144016
C	3.5109090555	1.739985783	-2.3182800926
C	4.0661950206	2.8125472526	-1.6164177664
H	2.2653464306	2.5089249202	1.2662003817
H	2.1042939615	0.0935896069	-2.2754758381
H	4.0511031275	3.9203192416	0.2372668583

H	3.8548499097	1.5129163661	-3.3231349449
H	4.8387885011	3.4230250856	-2.0736289965
H	4.8387885011	3.4230250856	-2.0736289965

TS 6-311++G(d,p) 0001

E(RB3LYP) = -1489.11931466 A.U.

First frequency = -265.6053 cm⁻¹

O	-1.7045154294	-2.0278977242	1.623325873
O	-0.2636621331	-2.7839020522	0.0521492877
O	0.8654634457	1.4760351589	0.8186873674
O	0.0761164466	0.1269102853	-0.9146278545
O	-2.5475350037	2.0197607085	-1.8672555566
O	-2.4517468173	-0.2164725026	-2.1366340449
N	-1.3056382304	0.8179398097	0.8243003009
N	-3.4545173814	0.827099868	1.0810106137
C	0.7416639968	-0.6589478571	2.89354669
C	-0.5793126169	-1.9861190191	1.1581267978
C	0.5657595824	-1.1413309479	1.4772980124
C	1.0889120681	-2.6296233419	-0.1980222578
C	1.8039736691	-3.3161837076	-1.1597810784
C	1.661462288	-1.7110959523	0.6890108053
C	3.0346635178	-1.4858656669	0.6271237846
C	3.7874227945	-2.1699042787	-0.3322567894
C	3.1809251461	-3.0649090094	-1.2202200804
C	0.0399334686	0.4717157532	0.2610754285
C	-1.4780947497	1.0919772257	-3.8279529372
C	-2.2153042376	1.0582084394	-2.5238607786
C	-2.9744996691	-0.4584236471	-0.8258106436
C	-4.5088959186	-0.2178412099	-0.732875401
C	-4.7843017134	0.3496123034	0.6777733179
C	-2.4654128879	0.4033782885	0.297294042
C	-1.5911239674	1.5395152421	1.9792734281
C	-2.9432637747	1.537567734	2.1453391108
H	-0.2174870937	-0.3698352762	3.3257449292
H	1.1660443395	-1.447998421	3.5237655744
H	1.4101595447	0.2008869062	2.934327649
H	1.3198930797	-4.0173014293	-1.8283901814

H	3.5096237501	-0.7775094531	1.2942793326
H	4.8561254309	-1.998607953	-0.3935491741
H	3.7822460676	-3.5786850813	-1.961513916
H	-0.4418320557	0.8089759835	-3.6249896786
H	-1.8947762448	0.3686274515	-4.5296268242
H	-1.5094669306	2.0961374601	-4.2453402453
H	-0.8098150414	1.9982613638	2.5550485794
H	-3.5634837323	1.97894927	2.9052783831
H	-2.7074529726	-1.4940016275	-0.6236090987
H	-5.0644348664	-1.1346449353	-0.9178997719
H	-4.7829305846	0.5160521541	-1.489390735
H	-5.1103160773	-0.4158671117	1.3827069818
H	-5.4968311584	1.1726998278	0.6824607586
C	2.1454346848	1.7093383682	0.3469794034
C	3.0982308787	2.0165342606	1.3193709295
C	2.4821202884	1.7259804809	-1.0080249724
C	4.4051025378	2.3110793553	0.9399424765
C	3.7976033164	2.010653047	-1.3723559636
C	4.7642417954	2.2983174975	-0.4084931274
H	2.8065383191	2.0150079169	2.362394445
H	1.7341727756	1.5001445253	-1.7514280687
H	5.1424491543	2.5438316329	1.6998825
H	4.0644452304	2.0108070097	-2.4233606294
H	5.7833067082	2.5179655964	-0.7048945342
H	5.7833067082	2.5179655964	-0.7048945342

TS 6-311++G(d,p) 0012

E(RB3LYP) = -1489.12169391 A.U.

First frequency = -253.3973 cm^{-1}

O	2.0014545521	-0.660703528	2.9849157136
O	0.2935239639	-2.0614108001	2.4592776222
O	0.9778326611	1.4336027727	0.9870500117
O	0.7573722373	0.5791064562	-1.1631404789
O	-2.2169333865	2.150352094	-1.6175212087
O	-1.5484573807	0.3489151433	-2.7971635082
N	-0.8609961313	0.2038442085	0.4609268012
N	-2.9334878144	-0.4042657643	0.357033663

C	2.8992216021	-1.0453474598	0.0323854659
C	1.405467684	-1.249950207	2.1066141225
C	1.5501589067	-1.2699844107	0.661038367
C	-0.1259714359	-2.7098162527	1.3179056725
C	-1.1649572164	-3.6158314306	1.241360931
C	0.6507438623	-2.3270000557	0.2130399388
C	0.4083362623	-2.9257588084	-1.021337168
C	-0.6280579094	-3.8636790722	-1.1231757842
C	-1.4129699034	-4.1925387345	-0.0142841643
C	0.5398018101	0.5005652723	0.0385885109
C	-0.8891688611	2.4495648307	-3.6174747494
C	-1.6319025131	1.680430953	-2.5672953289
C	-2.0488576502	-0.561006042	-1.8119623417
C	-3.5944094274	-0.7256166754	-1.8667272881
C	-4.0681697099	-0.9354606893	-0.4112095601
C	-1.8333352957	-0.2066241989	-0.3659328021
C	-1.3915007092	0.2902163509	1.7441112632
C	-2.6927383736	-0.1055190293	1.6809211254
H	2.7811550369	-0.7043781647	-0.9987969315
H	3.4633776518	-0.2889539798	0.5780092051
H	3.4845186189	-1.9714041427	0.0226227709
H	-1.751107601	-3.8746672849	2.1144592299
H	1.00304738	-2.6602836776	-1.8876278023
H	-0.8293337808	-4.3365405841	-2.0779406792
H	-2.2164209261	-4.9125604768	-0.1178295963
H	0.1798598172	2.2872271562	-3.4575189617
H	-1.1390685861	2.0820917703	-4.6136881711
H	-1.1186927375	3.5092860313	-3.5310543848
H	-0.7907396882	0.6163392942	2.5721916988
H	-3.4432517209	-0.1950001489	2.4460445126
H	-1.5321359158	-1.4925740806	-2.0317914897
H	-3.8805091341	-1.553811623	-2.5115171385
H	-4.0199524672	0.1935113411	-2.2672732371
H	-4.199969556	-1.9879693998	-0.1587758452
H	-4.9760186611	-0.3867961512	-0.1670099654
C	2.0653622388	2.2476133773	0.7021507852
C	2.0661133765	3.1069461305	-0.3954788897
C	3.1196145267	2.2348441922	1.6115818845

C	3.1548452864	3.9571519082	-0.5851471405
C	4.1973795237	3.097299154	1.4159763349
C	4.2210867127	3.95625963	0.3160717904
H	1.2312275163	3.1014472582	-1.0817926985
H	3.0783748053	1.5400103905	2.4410941678
H	3.1648852977	4.6269498933	-1.4377104062
H	5.0209830355	3.092510558	2.1210131479
H	5.0623847726	4.6223967275	0.1631897567
H	5.0623847726	4.6223967275	0.1631897567

TS 6-311++G(d,p) 0015

E(RB3LYP) = -1489.11810094 A.U.

First frequency = -274.4271 cm^{-1}

O	-1.7552864767	-2.0045935416	1.4210196841
O	-0.349909226	-2.5659178138	-0.2585367454
O	0.9200911648	1.4982242754	1.0534877945
O	0.0380703315	0.4089627197	-0.8137637717
O	-2.0914672464	1.4907630667	-3.7630332332
O	-2.8664109293	0.8033580846	-1.8313728499
N	-1.2703125596	0.9194553344	1.0311080129
N	-3.4201496872	0.8963784733	1.3028214176
C	0.7369144511	-0.8778445354	2.8416765251
C	-0.6312976256	-1.9305120741	0.95754596
C	0.5400209126	-1.1707431064	1.3778756158
C	1.0065269718	-2.4203284159	-0.4979372559
C	1.6915377297	-2.9820310196	-1.5572476822
C	1.6134677611	-1.6578406568	0.5061849427
C	2.9932260914	-1.4716179067	0.4639675397
C	3.7167781677	-2.0349530408	-0.5912847975
C	3.0758271187	-2.7701211122	-1.5941088036
C	0.0514617716	0.6035511424	0.3995346034
C	-1.5931012955	-0.7959977846	-3.2277140606
C	-2.1706950525	0.5721423773	-2.9823407909
C	-2.9186068853	-0.1456795991	-0.7465359087
C	-4.3875499536	-0.4453793635	-0.3539764022
C	-4.752387308	0.5306076566	0.7918481393
C	-2.4301359854	0.5304977946	0.4925329786

C	-1.5486526116	1.5464418042	2.2397138766
C	-2.9040515476	1.5367823696	2.4080385976
H	-0.2034245057	-0.5782440606	3.3073130531
H	1.1034645739	-1.7635391927	3.3713822402
H	1.4610240244	-0.0757655124	2.9839628182
H	1.1799406435	-3.5621196338	-2.3152723205
H	3.4956875254	-0.8826925968	1.2209690647
H	4.790269669	-1.8918462329	-0.6378092086
H	3.6555284101	-3.1896436065	-2.4082598766
H	-1.1650130019	-0.8059490703	-4.2272712873
H	-0.8160487002	-1.0112893058	-2.4931244433
H	-2.3648547479	-1.566255473	-3.1570298713
H	-0.7638821724	1.9475630933	2.8534137432
H	-3.5187489497	1.9244221361	3.2011121121
H	-2.3554095789	-1.0425849922	-0.9728750741
H	-4.4415815865	-1.4717495011	0.0083496509
H	-5.0444842453	-0.3395860529	-1.2150098982
H	-5.337634178	0.0618373096	1.5804337212
H	-5.2611464713	1.4310427786	0.4470809485
C	2.2109894265	1.7282928178	0.6051736232
C	3.1650641951	1.9158947538	1.6058823941
C	2.5581532132	1.8464087614	-0.7416479415
C	4.4847490239	2.1936646721	1.2596919468
C	3.8856111685	2.1149897434	-1.072944185
C	4.8537931259	2.2841965102	-0.0830897645
H	2.8643297226	1.8351443354	2.6432501663
H	1.8094443101	1.7096204172	-1.5057420154
H	5.2238182251	2.3331001223	2.0404703934
H	4.1606570551	2.1946383675	-2.1187256119
H	5.8822736359	2.4919723692	-0.3544047087
H	5.8822736359	2.4919723692	-0.3544047087

TS 6-311++G(d,p) 0016

E(RB3LYP) = -1489.11522619 A.U.

First frequency = -216.1896 cm^{-1}

O	1.507956253	-2.2363182785	-2.2831457057
O	2.5618726278	-2.2220641518	-0.2693673115

O	1.2101487529	0.4129703227	0.219120293
O	-0.2736088957	0.2220394347	-1.5550704528
O	-2.2971087086	2.7475266187	-0.6164565718
O	-2.9620187369	1.0259267446	-1.9109700466
N	-1.0169135471	0.1420262459	0.6406400789
N	-2.9638766463	0.3910812135	1.5505519671
C	-1.0934162461	-2.6690536143	-0.7015051465
C	1.3961122682	-2.2412698302	-1.0715797135
C	0.2414419683	-2.197974717	-0.2032740312
C	2.1628703195	-2.3662672541	1.0402313627
C	3.0016428639	-2.4614092177	2.131332838
C	0.7615533916	-2.4383427864	1.1306390589
C	0.1804486014	-2.6666393688	2.3784289356
C	1.0102848738	-2.774889134	3.5011728089
C	2.3983739059	-2.6612013337	3.3835408561
C	0.0368975878	-0.0083788106	-0.3995730455
C	-1.9544888729	2.8453732842	-3.0088130318
C	-2.4114047239	2.2488282992	-1.7133891418
C	-3.2912999013	0.2245089126	-0.7717616044
C	-4.6216741724	0.6584888267	-0.0886219901
C	-4.4262944912	0.4788482116	1.4344336304
C	-2.331640418	0.2502006357	0.3875070258
C	-0.8298238915	0.2527502697	2.0153971332
C	-2.0572510218	0.4013226319	2.5880929321
H	-1.347816185	-2.1627878957	-1.635250079
H	-1.0965918603	-3.747920279	-0.8916097611
H	-1.8783002355	-2.469391434	0.0330877997
H	4.077063164	-2.3942661823	2.0206769662
H	-0.8952713683	-2.7535118899	2.4793590211
H	0.5697959319	-2.9489476412	4.4765875465
H	3.0224218002	-2.7427505485	4.266069443
H	-1.7563428344	3.9068933778	-2.8770978314
H	-1.03280996	2.3328173295	-3.2971500049
H	-2.6927664522	2.6835038255	-3.7947398754
H	0.1528188505	0.2187978123	2.4448118441
H	-2.3495106787	0.5072775404	3.6177338739
H	-3.3521835446	-0.7834298867	-1.1786210284
H	-5.4625798737	0.0779048524	-0.4613869818

H	-4.7935334163	1.7083208312	-0.3203770945
H	-4.8668098815	-0.4444601267	1.8115039031
H	-4.7953787288	1.3195242104	2.0194411524
C	2.0993265679	1.2346076823	-0.4693476137
C	2.556320004	2.3487999522	0.2307822881
C	2.5676711709	0.9423297849	-1.7479394842
C	3.498006243	3.1898853972	-0.3597230349
C	3.5011598722	1.7996054536	-2.3309975164
C	3.9700301023	2.9204988085	-1.6448780924
H	2.170749979	2.5426469161	1.2243697549
H	2.2108168973	0.0661382183	-2.2693632141
H	3.8563984541	4.0566366238	0.1839123695
H	3.868495748	1.5807044069	-3.3273656849
H	4.6995205658	3.5761806902	-2.1060870208
H	4.6995205658	3.5761806902	-2.1060870208

5 Diels-Alder

5.1 Endo

5.1.1 Starting TS

TS endo input

E(RB3LYP) = -706.409984153 A.U.

First frequency = -508.8645 cm^{-1}

H	-1.7533835602	-0.3307583447	-2.1770495961
C	-1.3240993767	-0.8130791624	-1.3035963497
H	-0.6170048622	-1.5969641774	-1.5457130185
C	-2.0292809878	-0.8412806056	-0.1031238053
C	-1.3782329838	-1.3883390581	1.0261593403
C	-0.1313434184	-1.9839739555	0.9641935756
H	0.3550035073	-2.2870835416	1.8862765076
H	0.1708634734	-2.5464344037	0.0890143379
C	1.3033001712	-0.433456365	0.026438694
H	1.4807709643	-0.1023070357	1.0465078836
C	2.3499409765	-1.3503221063	-0.5760633565
C	0.5221907412	0.3808646769	-0.7900135963

H	0.743598111	0.3760512217	-1.8561476746
C	-0.0635512869	1.6566328777	-0.2367599532
C	-3.4388777875	-0.2166902028	-0.0045020391
H	-1.7868451042	-1.1882566333	2.0113606399
C	-4.4039553002	-1.1481482582	-0.779445496
C	-3.5083851606	1.1939914915	-0.6277196612
C	-3.940217536	-0.1089923859	1.4481379033
H	-3.9994917088	-1.0881835557	1.933363616
H	-4.9454422966	0.3248214245	1.4604956677
H	-3.2929838579	0.535559674	2.0522696632
H	-3.1576663173	1.2094228889	-1.6632319791
H	-2.9095889975	1.9076017311	-0.0565757146
H	-4.5449237854	1.5491788405	-0.6293487683
H	-4.1216635942	-1.2144234605	-1.8346952505
H	-5.4333915723	-0.7746231282	-0.7235888589
H	-4.3840202114	-2.1610029555	-0.3640558123
H	-0.5984240218	1.4221752267	0.6942101379
H	-0.8076944299	2.0593164964	-0.931110526
C	0.9905786876	2.7412422104	0.0483107972
H	1.7334263279	2.3510358504	0.7565749959
C	0.3797103604	4.0324752954	0.6041676456
H	1.5425965262	2.965882156	-0.8752319528
H	-0.1756048216	3.800717876	1.5235278448
H	-0.3624487022	4.4176820794	-0.1084998221
C	1.4247471988	5.113865065	0.8928818875
H	2.1600638787	4.7644801932	1.6267662353
H	0.9643827128	6.0247987195	1.2894222481
H	1.9720069005	5.3851795634	-0.0171931851
C	3.1742175494	-2.1367471854	0.4505120552
H	3.0279750818	-0.7448414335	-1.1929168092
H	1.8723323498	-2.0526782304	-1.2779624421
H	3.6657342484	-1.4256459534	1.1300073285
C	4.2338526747	-3.0622714966	-0.1668321262
H	2.5010061663	-2.7363569173	1.0729806853
C	5.3528646903	-2.3300963471	-0.9168469117
H	3.7401815269	-3.7711570953	-0.8459904396
H	4.678557793	-3.6682812238	0.6326715552
H	4.9730365354	-1.7853472684	-1.7869659004

H	6.1126658869	-3.031827834	-1.276013928
H	5.8511684674	-1.6039055193	-0.2639301612
H	5.8511684674	-1.6039055193	-0.2639301612

5.1.2 Lowest TS

TS endo 0008

E(RB3LYP) = -706.415808049 A.U.

First frequency = -505.0983 cm⁻¹

H	-1.895706556	-0.3941229586	-2.0892112311
C	-1.529840026	-1.0199381476	-1.2837428545
H	-0.8464658642	-1.7941283269	-1.610625562
C	-2.2673043633	-1.1897090853	-0.1167210011
C	-1.6719065011	-1.9281911174	0.9325302505
C	-0.4252941696	-2.5183670983	0.8248840091
H	0.0314036566	-2.9701191511	1.7012065071
H	-0.0957157631	-2.9403441866	-0.1167967795
C	1.0153017535	-0.8594158872	0.2441751858
H	1.0853212935	-0.6091795118	1.2990535425
C	2.1332988946	-1.7142478564	-0.3175832321
C	0.3250621551	0.0348672678	-0.5744747132
H	0.6273185262	0.0853312837	-1.6186519902
C	-0.2593904366	1.2960130967	0.0214221906
C	-3.6294831568	-0.503407252	0.1216506577
H	-2.1239211948	-1.8757731215	1.9201282189
C	-3.6340140305	0.3786330417	1.3912892467
C	-4.6826016915	-1.6252759817	0.2939682107
C	-4.0559459458	0.3803116332	-1.0642814883
H	-5.0343033529	0.8277595057	-0.8606195502
H	-4.1417145676	-0.1967637992	-1.990297778
H	-3.3468734338	1.197428549	-1.2337425263
H	-5.6797913405	-1.1974910485	0.4505137906
H	-4.4486110774	-2.2617490482	1.1528313184
H	-4.7186205427	-2.2640319106	-0.594447964
H	-3.3503942822	-0.1807435158	2.286708659
H	-4.6378083193	0.7835191467	1.5626950553
H	-2.9464991399	1.2225472011	1.288861306

H	-0.8570087504	1.0136927424	0.8954450476
H	-0.9470051049	1.7690246936	-0.6905818515
C	0.803021722	2.3221819032	0.4653904168
H	0.2979589388	3.1785508617	0.934049243
C	1.7042374965	2.8278257373	-0.6662562847
H	1.428517452	1.8707144965	1.2470179775
H	1.0837792608	3.3029100089	-1.4388115603
H	2.192800317	1.9732156271	-1.1496185952
C	2.7735163157	3.8094960986	-0.1795117
H	3.4332680744	3.3338273487	0.5553361181
H	2.3207329032	4.6846851196	0.300620568
H	3.3985473211	4.1672322903	-1.0044389034
C	3.4061737133	-0.9148987787	-0.6656635733
H	1.781673214	-2.2151352656	-1.2307664928
H	2.3907254122	-2.5114832199	0.3912292792
H	4.1448014739	-1.594810371	-1.1129986727
C	4.043807774	-0.1948771044	0.5274841384
H	3.1593292176	-0.1765718798	-1.4402347041
C	5.2775735797	0.6224357707	0.1352627542
H	4.3127870043	-0.9338671575	1.2948982322
H	3.3031578379	0.4692857066	0.9882624175
H	5.7245637689	1.1186875945	1.0029970846
H	5.0152389735	1.3986550548	-0.5928228962
H	6.0469127652	-0.0118060169	-0.3200836177
H	6.0469127652	-0.0118060169	-0.3200836177

5.1.3 Additional TS

TS endo 0001

E(RB3LYP) = -706.414690851 A.U.

First frequency = -508.4605 cm^{-1}

H	-1.6199133862	-0.6372306894	-2.1822833559
C	-1.3277644677	-1.143473892	-1.2697386594
H	-0.6281337466	-1.9549470911	-1.427409717
C	-2.1599913763	-1.1487702996	-0.1553734741
C	-1.6594707188	-1.7314043078	1.0319924012
C	-0.4086645451	-2.3165542011	1.1119049185

H	-0.0276609311	-2.6389576289	2.0770891766
H	0.0011391627	-2.8587443855	0.2680789439
C	1.0729108595	-0.7360034183	0.444228768
H	1.0426418641	-0.3214719666	1.4496796926
C	2.2525305268	-1.6330931701	0.1418561622
C	0.4690080478	0.0123560877	-0.5671989183
H	0.8754873909	-0.0936024817	-1.5726082404
C	-0.148204598	1.3515205808	-0.2427515434
C	-3.5255813153	-0.4296484599	-0.1228853184
H	-2.1915595659	-1.5441304594	1.961755816
C	-3.8668439141	0.2418403786	-1.4652615531
C	-3.5915224926	0.6543504294	0.9775485457
C	-4.6045791941	-1.5009119809	0.1686661573
H	-5.602308405	-1.0470566884	0.1879480064
H	-4.4355431138	-1.9854624362	1.1350321603
H	-4.5966021297	-2.2797823987	-0.6006850292
H	-2.8861322456	1.4646202169	0.7754401682
H	-3.3672665202	0.251549432	1.9689410995
H	-4.5974512577	1.0873745952	1.018994165
H	-4.8542945526	0.7111053891	-1.4048413643
H	-3.8923596549	-0.4824103552	-2.2855287822
H	-3.1449478539	1.0243308508	-1.7214673349
H	-0.7256571259	1.2526943094	0.6844886323
H	-0.8595438013	1.6502428548	-1.0222870276
C	0.8992162024	2.4644891034	-0.064424676
H	1.6011188975	2.17436073	0.7289045897
C	0.2768687329	3.8249863199	0.2685680896
H	1.4992181203	2.5508331813	-0.9815252392
H	-0.3239991724	3.7312198311	1.1836633405
H	-0.426146252	4.105833492	-0.5276417167
C	1.319260499	4.9321966566	0.4484271244
H	1.9119172962	5.0664398829	-0.4637524857
H	2.0150554882	4.6893654057	1.2597081683
H	0.8510063214	5.89291023	0.6865639868
C	3.5733508488	-0.8510378218	0.0284274775
H	2.0732920951	-2.1672938543	-0.8027176719
H	2.3617520078	-2.4044730577	0.9150692232
H	3.4738286707	-0.0941584579	-0.7610722728

C	4.7847989481	-1.744113679	-0.2607957648
H	3.7432799649	-0.2939947548	0.9606243719
C	6.0929159805	-0.9561947963	-0.3757635149
H	4.6076736055	-2.3024287199	-1.190344884
H	4.8767418275	-2.4981089453	0.5328889759
H	6.9432369523	-1.6139584616	-0.5834944908
H	6.3086490018	-0.414185383	0.5521069571
H	6.0372572139	-0.2169165366	-1.1829850944
H	6.0372572139	-0.2169165366	-1.1829850944

TS endo 0005

E(RB3LYP) = -706.414893150 A.U.

First frequency = -507.8112 cm⁻¹

H	-1.8097235766	-0.5783304237	-2.1999437041
C	-1.467419198	-1.1534095133	-1.3475561495
H	-0.8480294001	-2.0005892083	-1.615608722
C	-2.1881043997	-1.1677959919	-0.1577138385
C	-1.6199210169	-1.8502666129	0.9429122858
C	-0.4148630084	-2.5248277678	0.8686254705
H	0.0329358082	-2.9256428046	1.7738457305
H	-0.1280608216	-3.0440800605	-0.0378798999
C	1.1079047221	-1.0073584656	0.1257448401
H	1.1990976496	-0.6577661543	1.1505171131
C	2.1741272174	-1.9701269604	-0.352935712
C	0.460394617	-0.1620001552	-0.7763680913
H	0.7575444094	-0.2328411979	-1.8224024725
C	-0.020802186	1.194845838	-0.3205534322
C	-3.4889519421	-0.3622425908	0.0465325155
H	-2.0453746335	-1.6804971824	1.9292640964
C	-3.9080691186	0.406032252	-1.2197233799
C	-3.3710091084	0.6592092044	1.2011487468
C	-4.6093648142	-1.3740467327	0.3898524368
H	-4.730923062	-2.1067728352	-0.4144751896
H	-5.5654970243	-0.8565552046	0.5306535518
H	-4.38407026	-1.9228450559	1.3092501881
H	-2.631879159	1.4309196261	0.9706751945
H	-3.0822016125	0.1864986582	2.1437800796

H	-4.3346111452	1.1551335541	1.3643111566
H	-4.8487334275	0.9360536701	-1.0376924065
H	-4.0642839056	-0.2667769767	-2.0688169769
H	-3.1595485736	1.1518970728	-1.5068497479
H	-0.5099434817	1.0818617623	0.6545716038
H	-0.7809291382	1.5873775463	-1.0069560108
C	1.1192011802	2.2204163878	-0.1930820071
H	1.8665880278	1.8413443807	0.5167342565
C	0.6365014113	3.6027760089	0.2595974174
H	1.6383001993	2.3111704265	-1.1578219065
H	0.1128404616	3.5039955864	1.2204443967
H	-0.1093230892	3.9776577301	-0.4546703119
C	1.7749481345	4.6178110129	0.3957602001
H	2.5176141846	4.2798249542	1.1275593193
H	1.4069484151	5.5963833422	0.7211067127
H	2.2943510179	4.7568120733	-0.5593404188
C	3.5235144877	-1.2865504389	-0.6551128048
H	1.8219094834	-2.4680037405	-1.2672967261
H	2.3352846814	-2.7636249739	0.3881265286
H	4.2072721808	-2.0245680774	-1.0976926701
C	4.1937089633	-0.6592450335	0.572631524
H	3.3661455138	-0.510890925	-1.4166895189
C	5.5355541205	0.0002168091	0.242865794
H	4.3384453725	-1.4331000714	1.3393582789
H	3.521288341	0.0863932109	1.0143673733
H	5.4073541852	0.8006239434	-0.4948853692
H	6.2406048948	-0.7258594065	-0.1780899259
H	5.9991434205	0.4383906257	1.1328054296
H	5.9991434205	0.4383906257	1.1328054296

TS endo 0010

E(RB3LYP) = -706.414694895 A.U.

First frequency = -518.2033 cm^{-1}

H	-1.480388838	-0.8304824643	-2.1588092133
C	-1.2662691282	-1.2997125766	-1.2055734057
H	-0.6371393213	-2.1774940491	-1.2863912249
C	-2.142416364	-1.1678455201	-0.131358907

C	-1.7374596201	-1.7082619892	1.1097520132
C	-0.5422584729	-2.3867930751	1.2754965168
H	-0.2229637584	-2.6755267772	2.2732737973
H	-0.1591255569	-3.0216668044	0.4854044587
C	1.0981299574	-1.0024571075	0.571346445
H	1.0811723258	-0.5329761877	1.5532180269
C	2.1975484259	-2.0234590817	0.3663861604
C	0.5780937622	-0.2562780152	-0.4905723856
H	1.0010090628	-0.4308483406	-1.4780852881
C	0.042384977	1.1317205497	-0.228380284
C	-3.4473553721	-0.3461543474	-0.2067149134
H	-2.2856863125	-1.4185857673	2.0031452265
C	-3.6765243799	0.2647776857	-1.600857429
C	-3.4792850224	0.8052900937	0.82450448
C	-4.6174794357	-1.3145244833	0.0938555663
H	-4.6346959685	-2.1386126367	-0.6266866345
H	-5.5774010121	-0.788066039	0.0369404371
H	-4.5290638678	-1.7485609116	1.0943726061
H	-4.4513678175	1.3104327967	0.7934275471
H	-2.7082238769	1.549613849	0.6094314392
H	-3.3280846469	0.4490451449	1.8470570514
H	-2.884858188	0.9726099781	-1.8679263834
H	-4.6255290836	0.8107671014	-1.6150502334
H	-3.7239205411	-0.5047623412	-2.3777440308
H	-0.5746822412	1.0954070737	0.6777577145
H	-0.6198312243	1.4501361683	-1.042371181
C	1.1439053945	2.1887438503	-0.0373782221
H	1.8109741775	1.8734895119	0.7762382165
C	0.5865707425	3.5840231661	0.2658783957
H	1.7677065862	2.2350064856	-0.9412211898
H	-0.0368948217	3.5333821811	1.1691412183
H	-0.0843352109	3.890365685	-0.5484092177
C	1.6818652947	4.6373895799	0.4542090873
H	1.2600465675	5.6242335553	0.6711562661
H	2.2991037983	4.7286247513	-0.4469084691
H	2.3473926778	4.368933038	1.2826341337
C	3.6210876592	-1.430257724	0.4385429433
H	2.0618417534	-2.5148639346	-0.6079417659

H	2.1236962598	-2.8149127676	1.1222441481
H	3.7358301761	-0.8948602679	1.3918843359
C	3.9908960683	-0.492390952	-0.71514766
H	4.3424287578	-2.2589155801	0.4675388909
C	5.4220948036	0.0415627372	-0.6068215789
H	3.2889400802	0.3473737257	-0.7429419106
H	3.8662279834	-1.0273054848	-1.6671179332
H	6.1525955468	-0.7757115494	-0.6050932216
H	5.5600981881	0.6079221545	0.3215049917
H	5.6673249982	0.7066169869	-1.4413861652
H	5.6673249982	0.7066169869	-1.4413861652

TS endo 0015

E(RB3LYP) = -706.414062402 A.U.

First frequency = -521.2554 cm^{-1}

H	-1.6918991416	-0.7782687756	-2.1828683726
C	-1.3803209803	-1.1909131879	-1.2302849637
H	-0.6199829249	-1.957450201	-1.3183022329
C	-2.2386300959	-1.1862301084	-0.1338155337
C	-1.7210058341	-1.6380526773	1.1003505368
C	-0.4277881865	-2.1114759141	1.2408576962
H	-0.0418339147	-2.3299237888	2.2329483406
H	0.0327601286	-2.6894470657	0.4484284833
C	0.934394005	-0.4860235972	0.4715878757
H	0.8725888762	-0.0126055143	1.4478377043
C	2.1668184019	-1.3290949883	0.2215553014
C	0.2899205741	0.1543216549	-0.5913556581
H	0.7211325264	0.012500576	-1.5826242251
C	-0.4368333173	1.4654354768	-0.3891422536
C	-3.6567047707	-0.5781767242	-0.177196896
H	-2.2855984353	-1.4263687153	2.0054496126
C	-4.0287165944	-0.0549584621	-1.5761959517
C	-3.8208281615	0.5877488803	0.8246197252
C	-4.6546864886	-1.7010732498	0.1967516683
H	-5.6843719712	-1.3259305212	0.1679612925
H	-4.4644566313	-2.086688611	1.2028117797
H	-4.5755307404	-2.539987346	-0.5022420996

H	-3.170379496	1.4261428489	0.5625166191
H	-3.5860027029	0.2871297104	1.8493203271
H	-4.8556462709	0.9486934099	0.8167388359
H	-5.0530706946	0.3317647403	-1.5672632787
H	-3.9778832021	-0.8463296459	-2.3306840804
H	-3.3716904783	0.7618842577	-1.8926044927
H	-0.932576218	1.4466614893	0.5892451762
H	-1.2310001749	1.5713366256	-1.1362095169
C	0.4719357565	2.7104928975	-0.4763961265
H	1.0203982236	2.6889501272	-1.4291814531
C	1.4683282115	2.8746307138	0.6761303172
H	-0.1691210212	3.602421576	-0.5175161791
H	2.1333882642	2.0059481777	0.7125615744
H	0.9186284419	2.8794186179	1.6277342763
C	2.3041726877	4.1522062246	0.5560780937
H	2.8863384264	4.1542222798	-0.3727777476
H	3.0075307873	4.2527481514	1.3892734433
H	1.6674796659	5.0444716587	0.5467963752
C	3.4464321446	-0.4928801043	0.0427892957
H	2.0128051701	-1.9355726431	-0.6832509228
H	2.3224362031	-2.0397507866	1.0433412252
H	3.2982243295	0.2193065938	-0.7800401725
C	4.6927261763	-1.3424324655	-0.2292598654
H	3.61030922	0.1140043733	0.9442241808
C	5.9604341253	-0.5011479579	-0.4033950991
H	4.5259321543	-1.9494735756	-1.1296754883
H	4.8326632276	-2.0547459744	0.5952662266
H	5.8564703943	0.1981794053	-1.2408742058
H	6.8368709332	-1.1277178723	-0.5984078421
H	6.1663042407	0.090963377	0.4956370513
H	6.1663042407	0.090963377	0.4956370513

TS endo 0017

E(RB3LYP) = -706.414722049 A.U.

First frequency = -506.3276 cm^{-1}

H	-1.7310473524	-0.0296853867	-2.147332798
C	-1.4158455724	-0.7539721843	-1.4054918581

H	-0.6586832495	-1.4411476984	-1.7619113164
C	-2.2572430397	-1.1253557924	-0.362591486
C	-1.7305191469	-1.9856563614	0.6286557331
C	-0.4432872785	-2.4902076778	0.5785804822
H	-0.0527049447	-3.0477559414	1.425503655
H	0.0107319519	-2.7477333005	-0.3709404654
C	0.9358494709	-0.7031896616	0.4297157951
H	0.8658457075	-0.5899810463	1.5095896177
C	2.1784482694	-1.4052941424	-0.0715163325
C	0.2980814202	0.262990814	-0.3497818399
H	0.7168689033	0.4601831465	-1.334777908
C	-0.4154595073	1.4125535687	0.3245784965
C	-3.6716279347	-0.5363538652	-0.1743952373
H	-2.2847282829	-2.1025673819	1.5569188422
C	-4.6738102733	-1.7141151185	-0.2489749362
C	-4.0364267359	0.4756354964	-1.2753218927
C	-3.8376984694	0.1708817151	1.1901731398
H	-3.1888875659	1.0479257193	1.2612202369
H	-3.6053783719	-0.4892702174	2.03011187
H	-4.8728797507	0.5083358826	1.314857615
H	-5.0549034814	0.8451118395	-1.1169260943
H	-3.9984721864	0.0227309898	-2.2710161067
H	-3.3657745098	1.3412340494	-1.2667177448
H	-5.7025761122	-1.3522096041	-0.1370416487
H	-4.486044444	-2.4480931074	0.5405657747
H	-4.5946106845	-2.2312467492	-1.2106879893
H	-1.0359865828	1.0013735001	1.1288342339
H	-1.0983445213	1.9068437586	-0.3773690696
C	0.5428189666	2.462201542	0.9227730064
H	-0.0436961883	3.1996104598	1.4888338232
C	1.3944313241	3.1959248086	-0.1194530797
H	1.2050336527	1.9692533202	1.6473348709
H	0.7318454264	3.6808071748	-0.8499676158
H	1.9885766832	2.4663899901	-0.6839823259
C	2.3285309104	4.2369397579	0.5033414395
H	3.0233549622	3.7666978124	1.2087046077
H	1.7626025456	4.9961009622	1.0555294002
H	2.9239026612	4.7522359634	-0.2575983847

C	3.4447465938	-0.5449203425	0.0881443014
H	2.0525918238	-1.6600096645	-1.1339840228
H	2.3266821919	-2.3557916901	0.457126617
H	3.3134883594	0.3920928238	-0.4693582096
C	4.7222144633	-1.2488602109	-0.3820085954
H	3.553007163	-0.2553895402	1.1429212367
C	5.9731774635	-0.3795250834	-0.2252436965
H	4.6062371311	-1.5421247741	-1.4344577327
H	4.8490523352	-2.1835235117	0.1811542771
H	6.8727136996	-0.9011155709	-0.5681275423
H	6.128551379	-0.0991198632	0.8228443485
H	5.8831615482	0.5471545958	-0.803537736
H	5.8831615482	0.5471545958	-0.803537736

TS endo 0018

E(RB3LYP) = -706.414782834 A.U.

First frequency = -525.0055 cm⁻¹

H	-1.5658600764	-0.9711534207	-2.1551624289
C	-1.330988523	-1.3549196792	-1.1690504555
H	-0.6403859143	-2.1892453249	-1.1829786099
C	-2.2330552298	-1.2187518651	-0.1159811804
C	-1.8079146167	-1.6414566022	1.1621679582
C	-0.5629804432	-2.2053056619	1.3857113511
H	-0.2376708259	-2.3988668183	2.4043938248
H	-0.1188027552	-2.8614321458	0.6463764442
C	0.9555482947	-0.7382720617	0.6108584577
H	0.8677320712	-0.1953026575	1.5486698903
C	2.1440569781	-1.6750837283	0.518995679
C	0.4149961674	-0.1257678627	-0.526589074
H	0.8775914014	-0.3692861097	-1.4819527265
C	-0.2061574913	1.2527165127	-0.446335638
C	-3.5912959039	-0.499167588	-0.258008799
H	-2.3906907591	-1.3364720923	2.0282460232
C	-3.857298366	-0.0253758249	-1.6982106183
C	-3.6994226294	0.7298468464	0.6734698446
C	-4.6956773677	-1.5140316611	0.1256231885
H	-5.6877966354	-1.0579513702	0.0282189984

H	-4.5823869528	-1.8572762683	1.158278379
H	-4.6573865379	-2.3942238829	-0.5243010672
H	-3.5330253687	0.4683919611	1.7219985125
H	-4.6994101995	1.1722699645	0.599406974
H	-2.97143928	1.4973947655	0.3983279954
H	-4.844565273	0.4444268155	-1.7576726279
H	-3.8415827813	-0.8587244591	-2.4077073148
H	-3.1203560174	0.7157364074	-2.0248654787
H	-0.7608003145	1.336297296	0.4962727911
H	-0.9407428655	1.3768004294	-1.2492525447
C	0.8120432254	2.4105283113	-0.5441401213
H	1.4420882698	2.2585516192	-1.432332793
C	1.704814489	2.6025578848	0.6868782988
H	0.2613828971	3.3442885087	-0.7248730155
H	2.2228859068	1.666993349	0.918710094
H	1.0707093119	2.8226866097	1.5566840385
C	2.737528937	3.7173999371	0.499096133
H	2.2544133844	4.6751889144	0.2736950865
H	3.4144362279	3.4855226065	-0.3313893706
H	3.3488089758	3.854936342	1.3971583502
C	3.5114251467	-0.9565199674	0.5463770756
H	2.0696918082	-2.271545965	-0.4018864609
H	2.1226294074	-2.3904258626	1.3499030957
H	3.5412344543	-0.2848100991	1.4160848009
C	3.8542833333	-0.1656002097	-0.720675028
H	4.2982274161	-1.7042840504	0.7175511087
C	5.175707693	0.5986553227	-0.6010231499
H	3.0486453564	0.540379266	-0.9448697309
H	3.8986113518	-0.8576932788	-1.5729117999
H	6.0101985853	-0.0780137027	-0.3835916495
H	5.1276196218	1.3350820311	0.2094999372
H	5.4139258878	1.1365325568	-1.5245748
H	5.4139258878	1.1365325568	-1.5245748

TS endo 0027

E(RB3LYP) = -706.414214139 A.U.

First frequency = -510.5919 cm^{-1}

H	-1.7273455137	-0.5127679849	-2.1182284346
C	-1.4028884054	-1.0874449083	-1.2585704261
H	-0.8301568214	-1.9696438587	-1.5174640515
C	-2.1084664717	-1.0426567592	-0.0600915873
C	-1.5598024851	-1.7303879743	1.0467050127
C	-0.3900919667	-2.4651925599	0.9696725268
H	0.0499753299	-2.8702018371	1.8768511195
H	-0.1448009516	-3.0180930953	0.0708802452
C	1.1955837932	-1.0465194412	0.1731597373
H	1.3291428394	-0.6920597173	1.1916141806
C	2.1974355445	-2.0695404649	-0.3189638074
C	0.571886283	-0.1768647593	-0.7230605162
H	0.8461489586	-0.2646987172	-1.773933466
C	0.1508980528	1.1984640386	-0.2632632383
C	-3.3656218213	-0.1698090418	0.1422275805
H	-1.9625864208	-1.5207932306	2.0348901897
C	-3.1885910552	0.861777802	1.2801591959
C	-4.5314986932	-1.1200217304	0.5096127434
C	-3.7575391437	0.5998269056	-1.1320180379
H	-3.9541804825	-0.0763832239	-1.9698901468
H	-2.976128362	1.3040497526	-1.436675991
H	-4.6694043371	1.1780151223	-0.9501536657
H	-4.6960411978	-1.8573091246	-0.2828051985
H	-5.4598357068	-0.5542639858	0.6508506125
H	-4.3245540869	-1.6660115042	1.4349865234
H	-4.1257512929	1.4060899472	1.4428644448
H	-2.4149144669	1.5932985204	1.032699089
H	-2.9152019733	0.3900601723	2.2278435739
H	-0.3096447396	1.1066881453	0.7283012035
H	-0.6191126543	1.6010714253	-0.9289847425
C	1.3279228613	2.1873670832	-0.1757695836
H	2.1068049956	1.7508813302	0.462040608
C	0.9395306435	3.5692298806	0.3730186564
H	1.7791122776	2.3023552532	-1.1717094161
H	1.8504863192	4.1694250156	0.4934862895
H	0.5183313244	3.4486046354	1.3807414809
C	-0.0541807968	4.33904395	-0.5049538612
H	-1.0217378905	3.8306132268	-0.5668108551

H	0.3280859292	4.4479631048	-1.5267929374
H	-0.2369445889	5.3431469428	-0.1085519129
C	3.5753926488	-1.4641648544	-0.6565329788
H	1.7984371988	-2.5554737264	-1.2204655114
H	2.3312700238	-2.8641707378	0.426355216
H	4.2074066806	-2.2426541193	-1.1066248689
C	4.3058719778	-0.8654110431	0.5509088632
H	3.4447564197	-0.6872475047	-1.4218630902
C	5.6773474079	-0.2896382848	0.187915352
H	4.4204464693	-1.639014407	1.3229848122
H	3.6872620577	-0.0774136183	0.9979095417
H	5.5821346427	0.5088062118	-0.5569300885
H	6.3300734886	-1.0606126244	-0.2375645772
H	6.1832510372	0.1300244155	1.0636097314
H	6.1832510372	0.1300244155	1.0636097314

TS endo 0049

E(RB3LYP) = -706.414384248 A.U.

First frequency = -519.3805 cm^{-1}

H	-1.4687785132	-1.1543804782	-1.9915624505
C	-1.2397635138	-1.4281885962	-0.9681880428
H	-0.6454372617	-2.3295621811	-0.8838204656
C	-2.075101684	-1.0442993798	0.077842157
C	-1.6485443255	-1.3363095923	1.3926583361
C	-0.4745783964	-2.018619719	1.6633278481
H	-0.1324755994	-2.1113395564	2.6905878907
H	-0.1446702395	-2.8188870431	1.0114956676
C	1.1925193373	-0.8847489672	0.6482686062
H	1.2323584525	-0.2310041929	1.5176139211
C	2.2413215701	-1.9764831262	0.6164854027
C	0.6613350892	-0.3382197921	-0.5242216991
H	1.0430494156	-0.7165180612	-1.4706186845
C	0.1785172827	1.0930164563	-0.5168021308
C	-3.3516784102	-0.2013002288	-0.1311631932
H	-2.1548676653	-0.8465419966	2.2212169041
C	-3.300774215	1.1446487619	0.6281537577
C	-4.5431367525	-1.0306869382	0.4072520673

C	-3.6146386779	0.1071962113	-1.6161533439
H	-2.8103561198	0.7078590386	-2.0538019385
H	-4.5440354954	0.6771821755	-1.717650959
H	-3.7189289956	-0.8078676166	-2.2075681635
H	-4.6172722735	-1.9891334605	-0.1166230514
H	-5.485115992	-0.487989507	0.2659800485
H	-4.4323183925	-1.2423898589	1.4749911054
H	-4.2590391694	1.6675511471	0.5317693974
H	-2.5227165952	1.7959748788	0.2218201606
H	-3.1055953695	1.010911221	1.6955734729
H	-0.4077530065	1.2419203743	0.396079602
H	-0.5014599533	1.276990799	-1.357614481
C	1.3223573118	2.1227289721	-0.5683972597
H	1.9972705516	1.9538211344	0.2817298106
C	0.8438248313	3.5830671481	-0.5624422009
H	1.9195629109	1.9446404739	-1.4725816041
H	0.168803328	3.74502319	-1.4142354808
H	1.7079697644	4.2384667365	-0.7303023124
C	0.141547397	4.0048115594	0.7336962685
H	0.7885480651	3.8338175169	1.6021627248
H	-0.7844835268	3.4447810299	0.8978612093
H	-0.1178321308	5.0683383761	0.7151932067
C	3.6898073887	-1.449141231	0.5324870106
H	2.0502976828	-2.6405145553	-0.2389654302
H	2.1625071	-2.6020331592	1.5141107953
H	3.8630154553	-0.7499374786	1.3630082294
C	4.053642599	-0.7638631862	-0.788594833
H	4.3766324744	-2.2912277994	0.6968152404
C	5.5107803788	-0.2944699478	-0.8287556829
H	3.3894041085	0.0911889742	-0.9514408528
H	3.8658377014	-1.4598349515	-1.6182293419
H	6.2029252262	-1.1342557968	-0.6973620405
H	5.7128594243	0.4264371924	-0.0280888079
H	5.7510294099	0.1901548498	-1.7807804655
H	5.7510294099	0.1901548498	-1.7807804655

TS endo 0055

E(RB3LYP) = -706.413920777 A.U.

First frequency = $-507.4897 \text{ cm}^{-1}$

H	-1.5122907896	-0.111259101	-2.1714793067
C	-1.2228202023	-0.7917350341	-1.3794378026
H	-0.4162044171	-1.4603490543	-1.6532040663
C	-2.1214714396	-1.1562702388	-0.3828431566
C	-1.6336270499	-1.9537742057	0.6782580097
C	-0.32718025	-2.4052364373	0.7389990365
H	0.0238189883	-2.9121135623	1.6337534826
H	0.2021914353	-2.6816007229	-0.1651377681
C	0.9888132074	-0.5712051466	0.609807943
H	0.841575042	-0.418744806	1.6770673933
C	2.2884530446	-1.239801675	0.2197047317
C	0.3691703243	0.3369602796	-0.2501221401
H	0.847936808	0.5146490621	-1.2112219774
C	-0.4358533855	1.4794649517	0.3258947882
C	-3.5675266383	-0.6197490171	-0.318904142
H	-2.2474123762	-2.056974413	1.5699406853
C	-4.5152460059	-1.8402693271	-0.4149473982
C	-3.8915637985	0.333053429	-1.4836417297
C	-3.8584548515	0.1318171546	1.0002988188
H	-3.6618602114	-0.4854724498	1.8809644618
H	-4.9121770683	0.4306016206	1.0379045472
H	-3.2507456296	1.0370127423	1.0806334346
H	-3.7645374239	-0.1557885546	-2.4546542398
H	-3.2579034267	1.2259359725	-1.4639449883
H	-4.9325144255	0.6651336058	-1.4125351263
H	-4.347277332	-2.3901567721	-1.3466151361
H	-5.5626973304	-1.517630957	-0.3903187123
H	-4.3560351306	-2.5349417567	0.4153598214
H	-1.0902634984	1.073884916	1.1057840894
H	-1.0912217936	1.9127498123	-0.4396699292
C	0.434243935	2.5961369166	0.9371637516
H	-0.2203481726	3.3292288939	1.4294007978
C	1.3212222094	3.3229632546	-0.08007216
H	1.0669804292	2.1657144402	1.7251452778
H	0.6892737325	3.7391001169	-0.8771283688
H	1.9873325383	2.5988928707	-0.5658157671

C	2.1585718094	4.4382529724	0.5516372364
H	1.5195431525	5.1934724863	1.0236569445
H	2.7819622098	4.9459318785	-0.1917869428
H	2.8224609198	4.038179484	1.3266547226
C	3.5049665999	-0.3207746181	0.4431444934
H	2.2379958425	-1.5330534612	-0.8373358428
H	2.4368942108	-2.1657200874	0.7909314142
H	3.3904330278	0.5778153776	-0.1780854986
C	4.8594836433	-0.9821653986	0.1469360772
H	3.4926918375	0.027258795	1.4845642576
C	5.0558555914	-1.3697932389	-1.3232534395
H	4.9722945758	-1.873542718	0.7793952412
H	5.6601794677	-0.2936847097	0.4458382365
H	4.3366382196	-2.1306449621	-1.64299378
H	6.0586637797	-1.7736384159	-1.4963073923
H	4.9290468375	-0.4991857519	-1.9775278462
H	4.9290468375	-0.4991857519	-1.9775278462

TS endo 0057

E(RB3LYP) = -706.414830615 A.U.

First frequency = -509.2439 cm^{-1}

H	-1.7247971285	0.3829739775	-2.0094394648
C	-1.4179956232	-0.4854585989	-1.4382816364
H	-0.7629524379	-1.1540823479	-1.9836159914
C	-2.2074709717	-0.9753444467	-0.4023907324
C	-1.6869125614	-2.0400570764	0.368907535
C	-0.467488313	-2.6369176789	0.1015594941
H	-0.0639174461	-3.3669658042	0.797831674
H	-0.1286556825	-2.7609332929	-0.9197646316
C	1.0758917796	-0.9660118522	0.0877649775
H	1.1412348388	-1.0803467936	1.1661626614
C	2.1505613245	-1.6547235776	-0.7283207994
C	0.4453465503	0.1830789556	-0.3911441187
H	0.7789342768	0.5689301391	-1.3528257219
C	-0.1038391839	1.1955922219	0.5868770503
C	-3.5434009267	-0.3236146289	0.0144019254
H	-2.1708483193	-2.2765064412	1.3135967004

C	-4.6529307495	-1.3845323527	-0.1873849713
C	-3.890203616	0.9048439999	-0.8459956988
C	-3.5474374182	0.121919957	1.4947153461
H	-3.3176746499	-0.7013929675	2.1763338129
H	-4.5365123639	0.5067411622	1.7678362718
H	-2.8187892691	0.9179142045	1.6694090695
H	-4.8545481804	1.3173514532	-0.5317765115
H	-3.9690740184	0.6479410051	-1.9069905412
H	-3.1415251874	1.6969381127	-0.7398984345
H	-5.6335308541	-0.9720905202	0.077553348
H	-4.4775607311	-2.267063226	0.4353324568
H	-4.6897893372	-1.7145703419	-1.2306004959
H	-0.6978238146	0.6589842343	1.335256339
H	-0.7927274219	1.8791119603	0.0785369445
C	0.9854873815	2.0065453331	1.3213975998
H	0.4925002324	2.7205406069	1.9962291255
C	1.956728201	2.767264272	0.4058059193
H	1.5619212006	1.3245485999	1.9592476526
H	2.5299752155	2.0463195931	-0.189826429
H	2.6889032125	3.293353901	1.0314419961
C	1.2743353009	3.7713310299	-0.5291000789
H	2.0104156413	4.3383859945	-1.1081544328
H	0.6689165158	4.489275424	0.0366202038
H	0.6102175012	3.2712044242	-1.2420599724
C	3.4720990274	-0.863582421	-0.8081415029
H	1.781756309	-1.8116024197	-1.7520747668
H	2.3526115453	-2.6522584155	-0.3179778359
H	4.1762361927	-1.4078341549	-1.4530781215
C	4.1319736823	-0.6039435614	0.5503304008
H	3.2807905471	0.0972384192	-1.3045551801
C	5.4305652057	0.1983532033	0.4328013567
H	4.3296161927	-1.5643844459	1.0462789618
H	3.4296828256	-0.0639438811	1.1966271468
H	6.1631942647	-0.3214008225	-0.1953637055
H	5.8901056797	0.3673288566	1.4121176078
H	5.243129366	1.1785413747	-0.0207503499
H	5.243129366	1.1785413747	-0.0207503499

TS endo 0058

E(RB3LYP) = -706.413684228 A.U.

First frequency = -508.9713 cm^{-1}

H	-1.4033001789	-0.9052528422	-2.0655869231
C	-1.1096038602	-1.227461544	-1.0734536499
H	-0.3933257001	-2.0397246174	-1.0744831683
C	-1.9509792124	-1.0420920991	0.0185221808
C	-1.449525994	-1.3833336324	1.2958944641
C	-0.1895683654	-1.9214265362	1.4884257824
H	0.1897073172	-2.0514726164	2.4983481443
H	0.2331788826	-2.6064181533	0.7630740367
C	1.2721507959	-0.4730855632	0.5445283583
H	1.2367192978	0.11427865	1.4596933996
C	2.4639409437	-1.3933455299	0.4027117987
C	0.6577538293	0.074729881	-0.5827225314
H	1.0701747524	-0.1951171049	-1.5544518745
C	0.0068514793	1.4335830485	-0.4908287938
C	-3.3298901997	-0.3564662432	-0.0900765932
H	-1.9914480203	-1.0351480185	2.1721791668
C	-3.4218134384	0.9187104516	0.7794911911
C	-4.3902771817	-1.3716978479	0.4016646715
C	-3.6770380859	0.0364698585	-1.5372977691
H	-4.6734587596	0.4892846882	-1.5699993146
H	-3.684410884	-0.8328498807	-2.2023156377
H	-2.9688030479	0.7688836349	-1.9387476544
H	-4.3618916407	-2.285254178	-0.200990833
H	-5.3966007423	-0.9429970159	0.3287593457
H	-4.2190145945	-1.6551245098	1.4444867281
H	-2.7406008985	1.6921234908	0.4151520453
H	-3.1807973383	0.7235511672	1.8278741974
H	-4.4389922115	1.3251497781	0.74562028
H	-0.5751923395	1.4677223118	0.4360770472
H	-0.7047283945	1.5809290826	-1.3127809407
C	1.0308604863	2.5839044646	-0.5024730839
H	1.7148997991	2.4617320014	0.3482542504
C	0.3964867524	3.9825764343	-0.4578251709
H	1.6507215671	2.4968456495	-1.4049371705

H	-0.2774557949	4.1008743781	-1.3176309832
H	1.1868147677	4.7333946695	-0.5852113914
C	-0.3705286552	4.2787492112	0.8363451375
H	0.2746798384	4.1450514744	1.7126738879
H	-1.233968345	3.6172116854	0.9596618032
H	-0.7423357719	5.3084783023	0.8497750652
C	3.7732481632	-0.6167647873	0.1646598025
H	2.2870884267	-2.082046629	-0.4342032622
H	2.5820605624	-2.0183072904	1.2977570008
H	3.6762464797	-0.0330763179	-0.7607267982
C	5.0273149888	-1.5009795097	0.089466319
H	3.8958991294	0.1157020097	0.9735721493
C	5.0425761863	-2.4622849101	-1.1046928405
H	5.1219975599	-2.0738120886	1.0223182586
H	5.9120281736	-0.853485855	0.0390814257
H	4.2301455886	-3.1938727049	-1.0486336968
H	5.9832514729	-3.0204682345	-1.1523317585
H	4.9306412572	-1.9155262464	-2.0484105579
H	4.9306412572	-1.9155262464	-2.0484105579

TS endo 0061

E(RB3LYP) = -706.414772832 A.U.

First frequency = -509.0443 cm^{-1}

H	-1.9757797208	-0.2779058187	-2.0716427906
C	-1.5138351825	-0.9235216866	-1.3340088133
H	-0.8131979346	-1.6335279835	-1.7560681507
C	-2.1506195989	-1.2046591613	-0.1294531392
C	-1.434860334	-1.9598338245	0.8281874064
C	-0.1675916288	-2.4642104202	0.593691037
H	0.3811358755	-2.9332873953	1.4058902247
H	0.1081888499	-2.8182533068	-0.3922845948
C	1.1293763626	-0.702059625	0.0018987432
H	1.2851531466	-0.513803129	1.0609304273
C	2.2307446496	-1.4581058616	-0.7106530987
C	0.3233495458	0.202094209	-0.6911605866
H	0.5337651842	0.3447765864	-1.7491786633
C	-0.2891054469	1.3734286419	0.0429094014

C	-3.5302833166	-0.6220782148	0.2455828936
H	-1.811824228	-1.9895324367	1.8477128632
C	-3.4942759209	0.1866673833	1.5625667564
C	-4.4972626138	-1.8180040358	0.4250151426
C	-4.0972699413	0.2956244195	-0.8525217491
H	-4.2162408735	-0.2341722729	-1.8027998062
H	-3.4543726381	1.1655837889	-1.0230382472
H	-5.0833183883	0.6661162126	-0.5536962009
H	-4.5604241286	-2.4079677526	-0.495064878
H	-5.5042400634	-1.465413367	0.6771847574
H	-4.1613535509	-2.4841173238	1.2256149983
H	-3.1114382439	-0.4014974088	2.4008243175
H	-4.5054411593	0.5150698159	1.8282807845
H	-2.8690623863	1.0779043304	1.4622562885
H	-0.7933853073	0.9871372502	0.9357957092
H	-1.0623952122	1.8454115176	-0.5757009521
C	0.7349841737	2.4396172567	0.4809750641
H	0.2121454997	3.2250705782	1.0447262583
C	1.5092641751	3.0809425181	-0.6754121056
H	1.4472842135	1.9835002685	1.1815312943
H	0.7985323473	3.5435776889	-1.3742941636
H	2.0287146872	2.2977601478	-1.2411101932
C	2.5266822107	4.1222922147	-0.2019486695
H	3.2698871572	3.6665313418	0.4625944747
H	2.0378224387	4.9300965976	0.3547839805
H	3.0640961289	4.573341441	-1.042570107
C	3.4543822473	-0.5850820427	-1.0657525157
H	1.8334653317	-1.8820807581	-1.6436779617
H	2.5550683064	-2.3116927274	-0.1043674603
H	4.2054070519	-1.2196510818	-1.5570354293
C	4.1049247381	0.135585001	0.124986735
H	3.1469445595	0.1638075129	-1.806672165
C	4.5909084671	-0.8041287569	1.2333315251
H	3.3918222166	0.8555030251	0.5440504641
H	4.9508796491	0.7278753055	-0.2460735016
H	5.1122700618	-0.2512198865	2.0213968561
H	5.2836766876	-1.5565404731	0.8384174014
H	3.7579339263	-1.3378343307	1.7031624893

H 3.7579339263 -1.3378343307 1.7031624893

TS endo 0064

E(RB3LYP) = -706.413158809 A.U.

First frequency = -511.5058 cm⁻¹

H -1.4865404297 -0.3640040983 -2.1739731584
C -1.1655666332 -0.9262560941 -1.3048475943
H -0.4636815133 -1.718335389 -1.5349105818
C -1.9696430264 -1.0152705456 -0.1729268253
C -1.4326879732 -1.6689900012 0.9598736117
C -0.1750251749 -2.2457432132 0.9674673522
H 0.2349147127 -2.6266248236 1.898936327
H 0.2139678326 -2.7296233201 0.0794928322
C 1.2782214719 -0.6156131102 0.3578190356
H 1.2868701473 -0.2806059336 1.3928519698
C 2.4465796859 -1.4808722814 -0.0596317844
C 0.6280758189 0.2028154921 -0.567192491
H 0.9992054375 0.189095797 -1.5914709854
C -0.0051805326 1.4944518598 -0.1084191985
C -3.3411718646 -0.3155351202 -0.0596970121
H -1.941271449 -1.5489433147 1.9136051753
C -3.7222902607 0.4406076532 -1.3452057511
C -3.3930076642 0.6914981804 1.1122868995
C -4.4014764961 -1.4170810541 0.184097416
H -4.2040630347 -1.9628113767 1.1117069492
H -4.4031253326 -2.14278599 -0.6356250079
H -5.4034060035 -0.9780762452 0.2565603006
H -3.137589027 0.2271755131 2.0686058828
H -4.4032969521 1.1053655228 1.2076761484
H -2.7040694484 1.5240746383 0.9476310947
H -3.7599005896 -0.2266802919 -2.2119721481
H -3.0156291497 1.2478051688 -1.5651127054
H -4.7129598014 0.8924491368 -1.2298134084
H -0.5363448472 1.3039866281 0.832543822
H -0.7585083874 1.8248899407 -0.8305673578
C 1.0232396507 2.6176461461 0.1190157556
H 1.7980789144 2.2501999521 0.8035376718

C	0.4159982131	3.91067612	0.6853414274
H	1.5340518362	2.8378717832	-0.8293389467
H	1.2283396797	4.6155247333	0.9042404758
H	-0.0632351266	3.6888225415	1.6489826019
C	-0.598535152	4.5892617764	-0.2427185356
H	-0.9413112983	5.5417375926	0.174503728
H	-1.4835199325	3.9652895875	-0.4040640172
H	-0.15561041	4.7948877235	-1.2244175225
C	3.7571101113	-0.6786722673	-0.1738342393
H	2.2300380128	-1.943916214	-1.0338787817
H	2.5814147451	-2.3046735551	0.6503278723
H	3.5946883498	0.15119008	-0.8729054988
C	4.966995868	-1.5059035775	-0.6352822115
H	3.9800062258	-0.2174308146	0.7988277533
C	5.4008535817	-2.5926393765	0.3552959904
H	5.8103496413	-0.8259027052	-0.8110682216
H	4.7391981849	-1.9655089565	-1.6070779409
H	6.3037419314	-3.1062318722	0.0091615624
H	4.624739375	-3.3521980363	0.4930961986
H	5.6190790222	-2.1606051946	1.3390154393
H	5.6190790222	-2.1606051946	1.3390154393

TS endo 0072

E(RB3LYP) = -706.414485071 A.U.

First frequency = -527.4199 cm^{-1}

H	-1.4037021346	-0.4478734073	-2.1129606723
C	-1.1828930969	-1.0575431145	-1.244375046
H	-0.4705045155	-1.848819374	-1.4420118285
C	-2.1143689491	-1.2005636667	-0.2175766922
C	-1.7087352283	-1.9111548158	0.9331465039
C	-0.4578761259	-2.4954119362	1.0447965222
H	-0.1486256419	-2.9263366924	1.9933071638
H	0.0098716217	-2.9478395746	0.178552567
C	1.0693583558	-0.8810008089	0.6779843048
H	0.9834668453	-0.6049558685	1.7275795922
C	2.2663867013	-1.7459050467	0.335251158
C	0.5077981781	0.0018043326	-0.2525885143

H	0.9746624928	0.0549609265	-1.2331827579
C	-0.1844599581	1.2563352338	0.2354038827
C	-3.4926825752	-0.5054622041	-0.2298339621
H	-2.3187723643	-1.8362455452	1.8302287107
C	-3.7218512476	0.3226760841	-1.5070734251
C	-3.6915243681	0.431602537	0.9834845447
C	-4.5672986289	-1.6190963535	-0.1782495873
H	-4.466061829	-2.2967001158	-1.0321828961
H	-5.5735672662	-1.1846525691	-0.201612738
H	-4.4782350144	-2.2168896559	0.7338774798
H	-3.5542318211	-0.0890669696	1.93501614
H	-4.7074352047	0.842595788	0.9781347835
H	-2.9906684294	1.2698106575	0.953854732
H	-4.7212918067	0.7693482745	-1.4848295298
H	-3.653788241	-0.2949520647	-2.4081208007
H	-2.997776176	1.1392842891	-1.5965245841
H	-0.8021118025	0.9842012416	1.0987683005
H	-0.8704310452	1.6378889755	-0.5303938064
C	0.7818612761	2.3857264276	0.642915977
H	0.2127033226	3.1826548405	1.1416194097
C	1.5531305122	2.9929831269	-0.5357317954
H	1.4895430139	2.0017736249	1.3898509244
H	0.8362869896	3.4417118286	-1.2369915075
H	2.0640618818	2.1986586953	-1.09282637
C	2.5791467689	4.0413044091	-0.0981967619
H	3.1005646584	4.4786341038	-0.9559570472
H	3.334431261	3.595926854	0.559672801
H	2.1006793227	4.8579113486	0.4546724557
C	3.6193594614	-1.1495232905	0.7836241279
H	2.279363561	-1.9340972956	-0.7463448537
H	2.1791912393	-2.7311007442	0.8102581251
H	3.5972616252	-1.0326788887	1.8756176809
C	4.0095127684	0.1937157339	0.1516563083
H	4.4061423815	-1.8870057005	0.5714614428
C	4.1871661547	0.1469714173	-1.3688932283
H	4.9469035009	0.5330936554	0.6106879826
H	3.2557470931	0.9446399527	0.4071596077
H	4.5193193129	1.1155374382	-1.7567876669

H	3.2522695655	-0.1060185937	-1.8789095629
H	4.9328936476	-0.6031584264	-1.6572995396
H	4.9328936476	-0.6031584264	-1.6572995396

TS endo 0073

E(RB3LYP) = -706.414115377 A.U.

First frequency = -530.9569 cm⁻¹

H	-1.8870126828	-0.5700348004	-2.2566548843
C	-1.5060869251	-1.0782887885	-1.378245774
H	-0.8401239172	-1.9008426989	-1.6099289919
C	-2.2313744722	-1.0863058664	-0.1880182707
C	-1.6196854334	-1.6711991003	0.9415730996
C	-0.3663710243	-2.257610886	0.8910744002
H	0.1123983237	-2.5804864	1.8117076443
H	-0.0590429967	-2.8132123065	0.0130890836
C	1.0359231848	-0.7002307403	0.0649481956
H	1.1271357157	-0.3029001336	1.0711937186
C	2.1408768862	-1.6334620526	-0.3916977623
C	0.3303649267	0.0722041773	-0.8658027347
H	0.6304640337	-0.0255937818	-1.9096807459
C	-0.2465416233	1.4213496238	-0.4899971998
C	-3.5818291321	-0.3584013031	-0.0184445637
H	-2.0541602839	-1.4827232021	1.9205777039
C	-4.6303983971	-1.4167129843	0.4026171074
C	-4.064703577	0.2972048723	-1.3248113737
C	-3.5171362784	0.7383010562	1.0694759637
H	-2.8185196491	1.5307607095	0.7894346329
H	-3.2020799963	0.3395100797	2.0375904852
H	-4.5052711492	1.1920954799	1.2067241484
H	-4.1738601728	-0.4371491071	-2.129142632
H	-3.3784352555	1.0788012445	-1.6670742136
H	-5.0417487435	0.7651255566	-1.1656306255
H	-4.3606489895	-1.8921914499	1.3503222803
H	-4.7133348852	-2.2040579558	-0.3535871016
H	-5.6163379238	-0.9535278289	0.5258502917
H	-0.5281348226	1.404056853	0.5687947688
H	-1.1724842911	1.6030129646	-1.0455197418

C	0.6949908091	2.6136022001	-0.770933106
H	0.9237340671	2.6267737926	-1.8454109988
C	2.0134014334	2.6420449472	0.0145014707
H	0.1395256265	3.5399667873	-0.567067012
H	2.6058518364	3.4977447667	-0.3341146125
H	2.5972233904	1.7490886933	-0.2274341287
C	1.8396288126	2.7418148735	1.5329743282
H	1.2537418419	3.6272522953	1.8063247055
H	2.809099398	2.8133751808	2.0370137383
H	1.3221659371	1.8677244593	1.9406566395
C	3.4946363423	-0.9329110962	-0.6237236453
H	1.8274478181	-2.1176484673	-1.3270259336
H	2.2893582656	-2.4407177259	0.3372362509
H	4.1831324706	-1.6343167207	-1.1152349705
C	4.151596672	-0.418456241	0.663573534
H	3.3517951603	-0.1005408801	-1.3256674531
C	5.4382660513	0.3676119532	0.3992400274
H	4.3637967894	-1.2727200059	1.3208462273
H	3.4468211038	0.217526621	1.2121531925
H	5.9040792677	0.7039686938	1.3312478636
H	5.2336170287	1.2550734575	-0.2107130089
H	6.1718862888	-0.2419755823	-0.140799956
H	6.1718862888	-0.2419755823	-0.140799956

TS endo 0081

E(RB3LYP) = -706.414094593 A.U.

First frequency = -525.9540 cm⁻¹

H	-1.4877343547	-1.2071834001	-2.0776640139
C	-1.2642684216	-1.4264706852	-1.0399532615
H	-0.6038671539	-2.2751049367	-0.9100037111
C	-2.1576465393	-1.0798809679	-0.0282972984
C	-1.7441655678	-1.2932509725	1.3045039769
C	-0.5223305877	-1.862063265	1.6246148557
H	-0.2011497547	-1.8920730327	2.662423604
H	-0.1126111128	-2.655880002	1.011105166
C	1.0563636998	-0.6239462964	0.614163262
H	1.0109133764	0.0589689615	1.4583374192

C	2.192614874	-1.626072231	0.6574295575
C	0.5265994783	-0.1698981711	-0.6002083471
H	0.970248348	-0.5689084985	-1.5109619424
C	-0.0638114938	1.217958938	-0.7154984153
C	-3.4923621119	-0.3518486551	-0.2960432399
H	-2.3114695448	-0.8225818837	2.1040679815
C	-3.7381006756	-0.108405189	-1.7959331928
C	-3.5704615754	1.013660926	0.4245776016
C	-4.6272863658	-1.2606184757	0.2362711547
H	-4.5278596484	-1.4349895193	1.3118472988
H	-4.6108254892	-2.2351756605	-0.2623006548
H	-5.6056775398	-0.7995577691	0.0573456578
H	-3.4124738548	0.921542215	1.5025230198
H	-4.5590787045	1.4622870554	0.2746610184
H	-2.8238993897	1.7095687363	0.0332343647
H	-2.9752706961	0.5454859637	-2.2312697355
H	-4.7087674586	0.3777967942	-1.9385703169
H	-3.7488062956	-1.0452784452	-2.3617912403
H	-0.6611553583	1.417898664	0.1803189747
H	-0.7613318943	1.2539813856	-1.5594579957
C	0.9741838926	2.3463401781	-0.9148229946
H	1.5918952378	2.1037384842	-1.7900788031
C	1.8918333044	2.6481400191	0.2801947372
H	0.4294386747	3.2652544793	-1.1741554592
H	2.6171671289	3.412251467	-0.0274637673
H	2.478046129	1.7581457618	0.5314774984
C	1.1488398761	3.1383006972	1.5277335219
H	0.5423135303	4.0234998276	1.3028692098
H	1.8494718714	3.4072053275	2.3249880619
H	0.4751181883	2.373673256	1.9279639067
C	3.5969185548	-0.9938762164	0.5430247412
H	2.0631592225	-2.359687079	-0.1516447554
H	2.1540106	-2.194044399	1.5947598323
H	3.6922131005	-0.1999360599	1.2974242365
C	3.943599837	-0.4285927369	-0.8384413542
H	4.3451454801	-1.7533472658	0.8094888563
C	5.3312101586	0.217469078	-0.8798512467
H	3.1910825209	0.3091565733	-1.1352453635

H	3.8868080138	-1.2373441455	-1.5801781068
H	5.3913875049	1.0576461777	-0.1783807059
H	5.5670893307	0.6002442874	-1.8781645279
H	6.1127980688	-0.4995538885	-0.6032741299
H	6.1127980688	-0.4995538885	-0.6032741299

TS endo 0082

E(RB3LYP) = -706.414393894 A.U.

First frequency = -519.4031 cm^{-1}

H	-1.2254682803	-1.0836994103	-2.0378140758
C	-1.0522088726	-1.4176141032	-1.021351339
H	-0.3845615915	-2.2676097482	-0.9529237516
C	-1.9987126975	-1.1937468641	-0.0244924529
C	-1.6500752371	-1.5527067422	1.2966863672
C	-0.4421348046	-2.1499357907	1.614918728
H	-0.1735198335	-2.2947250151	2.6578872319
H	0.009754015	-2.8641903806	0.9368999383
C	1.1872118026	-0.7997754034	0.8272055411
H	1.1044674778	-0.2174430904	1.7431256584
C	2.3253923344	-1.7976269409	0.7978868555
C	0.6978495478	-0.2057035056	-0.3405018972
H	1.1797634866	-0.4712371469	-1.2792042384
C	0.0873078145	1.1741494017	-0.2697211397
C	-3.3288543613	-0.4524230496	-0.279335559
H	-2.2627702469	-1.1776341197	2.1131064178
C	-3.4739755948	0.8158731732	0.5927482752
C	-4.474671009	-1.4318638473	0.0743796282
C	-3.494028337	-0.0325506935	-1.7509989192
H	-2.7166289257	0.673890582	-2.060311876
H	-4.4617490411	0.4606415614	-1.8895628955
H	-3.4606890334	-0.8946295873	-2.4245662257
H	-5.4500205336	-0.9644001409	-0.1045816987
H	-4.4318162323	-1.7325451909	1.1255659083
H	-4.4120272349	-2.3393880968	-0.5347818295
H	-2.7222448307	1.5644355815	0.3295635224
H	-3.3737866491	0.598034701	1.6594718466
H	-4.4621900348	1.2647388521	0.4410500277

H	-0.5812047163	1.2080457117	0.5993190475
H	-0.5383053276	1.3640366397	-1.1501121029
C	1.1255927481	2.3020423167	-0.1418973932
H	1.7546442282	2.1170188091	0.7391111363
C	0.4869208374	3.6913523742	-0.0349794785
H	1.8012187125	2.2778906279	-1.0085903406
H	-0.1892186943	3.7102087517	0.8308348577
H	-0.1447240803	3.8678837806	-0.9163896302
C	1.5185869842	4.8156925791	0.0924334743
H	2.1865103453	4.837125591	-0.7763214775
H	2.142199512	4.6780433081	0.983172446
H	1.0389849962	5.7970083046	0.1689968751
C	3.7266622918	-1.1486293396	0.8610332703
H	2.2433185574	-2.4177783223	-0.1046457219
H	2.243840098	-2.4880567788	1.6462887335
H	3.7814683235	-0.5354285199	1.7705860703
C	4.1237579919	-0.2865762604	-0.3464611526
H	4.4707048438	-1.9479885349	0.9857071493
C	4.2278190035	-1.0646747652	-1.6625098782
H	5.092530751	0.182426799	-0.1319738588
H	3.4067065112	0.5334393796	-0.4608137685
H	4.576289666	-0.4203577639	-2.4762854275
H	3.262553009	-1.4821826496	-1.9671086705
H	4.9322869332	-1.8999679865	-1.5724390074
H	4.9322869332	-1.8999679865	-1.5724390074

TS endo 0084

E(RB3LYP) = -706.414073801 A.U.

First frequency = -513.3395 cm⁻¹

H	-1.798754678	-0.6424369127	-2.1897063061
C	-1.3789791966	-1.1370817692	-1.3215815692
H	-0.7671101338	-1.9968118532	-1.5658164109
C	-2.004075258	-1.057095194	-0.0807562865
C	-1.3365606207	-1.6316886476	1.0250383614
C	-0.1294243948	-2.2980502847	0.9092200601
H	0.3981141183	-2.6126161642	1.8056566885
H	0.0849804481	-2.8983765645	0.0332163435

C	1.3041247829	-0.8538629122	-0.0888782902
H	1.4936373068	-0.4282572557	0.8931796969
C	2.323517335	-1.8523098949	-0.5934624628
C	0.5664657225	-0.0767337053	-0.984237857
H	0.7724564376	-0.2110674323	-2.0457103323
C	0.0893339233	1.294145408	-0.5691371683
C	-3.3019650991	-0.2553949696	0.1564503938
H	-1.6831645563	-1.3794532805	2.0245731127
C	-3.8404148704	0.3848739525	-1.1356435414
C	-3.1149947602	0.8714789617	1.1984976972
C	-4.3671419763	-1.2479496503	0.6830162528
H	-4.5347889486	-2.055535729	-0.0368974705
H	-5.3210669482	-0.7349953426	0.8524187038
H	-4.0563452632	-1.7033598356	1.6280918994
H	-2.4263455881	1.6363319638	0.8302756613
H	-2.7259702355	0.4965524439	2.1489675765
H	-4.0756666901	1.3568695725	1.4045855294
H	-3.1354481552	1.1125404401	-1.5511927441
H	-4.7753032475	0.9147247723	-0.9254214081
H	-4.0491473428	-0.3666332346	-1.9035458464
H	-0.3178547935	1.2178070072	0.4445069954
H	-0.7341534672	1.628510765	-1.2124176257
C	1.2075071933	2.3526481359	-0.6002622367
H	2.0034910579	2.0536076956	0.0948197636
C	0.7308973582	3.7713473369	-0.2527524491
H	1.6630131841	2.3584806741	-1.5995090416
H	-0.0585378867	4.069278104	-0.9566444516
H	1.5606985671	4.4718348123	-0.4117213919
C	0.2176098246	3.9219717978	1.1841087917
H	-0.0440097193	4.9620239003	1.4044773715
H	0.9806715967	3.6091370811	1.9066282297
H	-0.6748835619	3.3143791671	1.3645844847
C	3.6498089743	-1.2031474543	-1.0441796557
H	1.8992615888	-2.3973461245	-1.4482949276
H	2.531488511	-2.6071990313	0.1736044133
H	4.3167137271	-1.9928069739	-1.4181386562
C	4.3816011977	-0.4041299543	0.0457552222
H	3.4429840243	-0.538295774	-1.8924079885

C	4.7490445039	-1.2278946112	1.2846752066
H	3.7623446198	0.4497474641	0.3465762334
H	5.2943850943	0.0221230906	-0.3892082139
H	5.3421953007	-2.1087061353	1.0118564292
H	3.857880019	-1.5820632198	1.813587896
H	5.3370920073	-0.6360500794	1.9935824755
H	5.3370920073	-0.6360500794	1.9935824755

TS endo 0095

E(RB3LYP) = -706.413085871 A.U.

First frequency = -522.7410 cm⁻¹

H	-1.4706831328	-1.1946639294	-2.0079515791
C	-1.1636265999	-1.3414132309	-0.978901925
H	-0.379815898	-2.0799141442	-0.8620571678
C	-2.0411045561	-1.0862172334	0.0720624003
C	-1.5322442612	-1.1913863577	1.3853645905
C	-0.228759524	-1.5732702948	1.6537846624
H	0.1465408622	-1.5195261555	2.6722383054
H	0.2587431346	-2.3218842738	1.0405523195
C	1.102711518	-0.1618212734	0.508956875
H	1.020010585	0.5353292528	1.3381439506
C	2.3563722652	-1.0102700848	0.4808138288
C	0.4535051688	0.1762352582	-0.683126906
H	0.9039238008	-0.1896638357	-1.6061200334
C	-0.3256610606	1.4657358037	-0.8112122914
C	-3.4765301348	-0.5591300305	-0.1386833326
H	-2.1179862516	-0.7742228976	2.2012305627
C	-3.7006103429	0.8123803897	0.5387855776
C	-4.4448225638	-1.5897857744	0.4914715122
C	-3.8362771958	-0.4141212903	-1.6283209818
H	-3.7471474489	-1.3663042881	-2.1607706368
H	-3.1976539468	0.3197880644	-2.1308675217
H	-4.8717044422	-0.072284961	-1.7282044184
H	-4.2632227199	-1.7048613092	1.5642583555
H	-4.3228625324	-2.572926492	0.0254413428
H	-5.4855188355	-1.2724751849	0.3569460116
H	-3.0758346019	1.5842931699	0.0821556582

H	-3.4752930889	0.786093923	1.6083771573
H	-4.7472298297	1.1191554697	0.4309828299
H	-0.8631681819	1.6456479431	0.1259649934
H	-1.0931579801	1.3613099761	-1.5859234786
C	0.5375820667	2.6966606829	-1.1687776781
H	1.0859553792	2.4802863654	-2.0956727643
C	1.5338144063	3.1612859278	-0.0959277379
H	-0.1397363634	3.5301842793	-1.4031344262
H	2.1247788778	3.9887014044	-0.5092816545
H	2.2449113818	2.3561170998	0.1166717397
C	0.875352126	3.6228168891	1.20864545
H	0.1484945838	4.4221485413	1.0218499086
H	1.6201497664	4.0069379968	1.9133758684
H	0.3424579563	2.8070269439	1.7077995158
C	3.6204205537	-0.2033821153	0.1290472772
H	2.2213012929	-1.8160063047	-0.2533029949
H	2.5143715503	-1.5006487679	1.4503162063
H	3.4822244781	0.267053021	-0.8538474298
C	4.9153648812	-1.030587551	0.1271138326
H	3.7217437743	0.618587098	0.8498565568
C	4.9657336525	-2.1104807725	-0.9599426606
H	5.0479973362	-1.4963251699	1.1134018305
H	5.7665239307	-0.3505244931	-0.0048902372
H	4.1915305964	-2.8708056951	-0.815559605
H	5.9324595434	-2.6243747567	-0.9630283614
H	4.817521595	-1.6720664648	-1.9538521277
H	4.817521595	-1.6720664648	-1.9538521277

TS endo 0099

E(RB3LYP) = -706.413177900 A.U.

First frequency = -512.4471 cm⁻¹

H	-1.6106488941	0.0316271401	-2.0142176015
C	-1.2591728367	-0.6672627333	-1.264143585
H	-0.4927546367	-1.3419877066	-1.6252102731
C	-2.0718321528	-1.043071115	-0.1990448551
C	-1.5014156338	-1.8669743296	0.7982120004
C	-0.2018924028	-2.3375237259	0.7298310089

H	0.2232296655	-2.8646170279	1.5796536086
H	0.2357749758	-2.6058400796	-0.2242825731
C	1.1304198567	-0.5180423423	0.4939138258
H	1.1058927513	-0.3977769396	1.574897194
C	2.3615344908	-1.2005069099	-0.0602778854
C	0.4268260539	0.4197874837	-0.264114172
H	0.804673961	0.635314592	-1.2620846757
C	-0.3102521863	1.5392444127	0.4338376295
C	-3.4988749064	-0.4905726931	0.0037307929
H	-2.0327744816	-1.9794041315	1.7403340012
C	-3.6597245142	0.2408615486	1.3560959555
C	-4.4678312946	-1.6977618663	-0.0267183236
C	-3.9137667407	0.4861815511	-1.1113673373
H	-3.8801553887	0.0130873331	-2.0977957422
H	-3.270100546	1.3718252819	-1.134235073
H	-4.9399113298	0.8284259223	-0.9417200289
H	-4.3920802088	-2.2328585285	-0.9788491453
H	-5.5043370138	-1.363136231	0.0979753974
H	-4.2436873214	-2.4090811436	0.7739642196
H	-3.034416544	1.1365150214	1.3966907658
H	-3.3935671499	-0.3949205933	2.2047922462
H	-4.7015757367	0.5518620673	1.4934807072
H	-0.8458884071	1.112591463	1.2894713008
H	-1.0745681626	1.9656006847	-0.2245653602
C	0.6171575437	2.6620064053	0.9448905007
H	0.0062862909	3.4039961135	1.4783947819
C	1.429818295	3.3759109368	-0.1468501778
H	1.3099726795	2.237239141	1.682430451
H	2.1143182918	2.659015547	-0.6173700992
H	2.0656008908	4.1329426651	0.3294471241
C	0.5723431511	4.0439996691	-1.2272671467
H	1.1918907616	4.6036612214	-1.9355283146
H	-0.1448688207	4.7449018759	-0.7840467152
H	0.000289925	3.3080729648	-1.8021423637
C	3.6145885404	-0.3071842686	0.0136807116
H	2.1864773119	-1.475800979	-1.1110080931
H	2.5485348904	-2.1372263927	0.4768215401
H	3.4079447479	0.6251349817	-0.5261650707

C	4.8864429451	-0.9531615811	-0.5575016521
H	3.7888589214	-0.0200770188	1.0603128139
C	5.3825939763	-2.1710192664	0.2306671386
H	5.6817727576	-0.1973452325	-0.5841445776
H	4.7056910695	-1.2413634132	-1.6023777472
H	5.5564565311	-1.9122962099	1.2817505505
H	6.3241780228	-2.550726496	-0.1792230433
H	4.6606071448	-2.9934951014	0.2080563196
H	4.6606071448	-2.9934951014	0.2080563196

TS endo 0105

E(RB3LYP) = -706.413257241 A.U.

First frequency = -528.3666 cm⁻¹

H	-1.4889686453	-0.1406162633	-2.0079989286
C	-1.2692714891	-0.8520181612	-1.2201227906
H	-0.6392679709	-1.6718989192	-1.5425522405
C	-2.1485672062	-1.0278040643	-0.1528607375
C	-1.7377882611	-1.8826018977	0.8930538461
C	-0.5360440989	-2.5703053309	0.8645531169
H	-0.209090807	-3.1176330129	1.7446231028
H	-0.1578856688	-2.9664674717	-0.0702889277
C	1.0968313002	-1.0444184828	0.5467509695
H	1.1039210743	-0.8766922897	1.6222877507
C	2.1839404592	-1.966305634	0.032378358
C	0.5507211991	-0.0275359672	-0.2457618994
H	0.960855502	0.0992717818	-1.2454471857
C	-0.0067693855	1.2115919748	0.4212724316
C	-3.4600650311	-0.2272975999	-0.0035326186
H	-2.285859061	-1.8526603755	1.8318215436
C	-3.5024027337	0.5947581087	1.3051159331
C	-4.6220804481	-1.2505221281	0.0154026049
C	-3.6947776813	0.7412301587	-1.1769236074
H	-3.73368153	0.2142600295	-2.1354496252
H	-2.9114400867	1.5040742217	-1.2379249413
H	-4.6495630164	1.2603411449	-1.0436408229
H	-5.586429423	-0.7366902283	0.1041765226
H	-4.5294335065	-1.9431827973	0.8573449936

H	-4.6326616716	-1.8437565181	-0.9046911524
H	-4.4763940395	1.0864049582	1.408453621
H	-2.7326548581	1.3705849542	1.3097244261
H	-3.3558357308	-0.0301489245	2.1901955508
H	-0.5169225364	0.8973538358	1.3390214163
H	-0.7738764569	1.674754456	-0.2069959396
C	1.0590577285	2.267479751	0.7803575178
H	0.5921757307	3.0362644423	1.4121444882
C	1.7120230842	2.9594893664	-0.4281753231
H	1.8356696646	1.7926122501	1.3933910143
H	2.1896272364	2.2105720271	-1.0715553073
H	2.5218505256	3.6053655345	-0.0656893162
C	0.7391771968	3.7979419079	-1.2654980675
H	1.2627232885	4.3246179548	-2.0699834016
H	0.2339438242	4.5492911794	-0.6473393255
H	-0.0353986887	3.1791297599	-1.7303558998
C	3.6179738685	-1.476432487	0.3234003688
H	2.0619814563	-2.100693247	-1.0521129243
H	2.07854818	-2.9632085717	0.4779423326
H	3.7326729071	-1.3339747193	1.4074833723
C	4.0183639157	-0.1869741335	-0.3982159556
H	4.3202336946	-2.2751899161	0.0466160959
C	5.4666179697	0.225166712	-0.1208307253
H	3.3444006057	0.6192565072	-0.0945898727
H	3.8706601381	-0.3173224105	-1.4795855933
H	5.7266473663	1.1525280703	-0.6416823636
H	6.1700761054	-0.5498820619	-0.4463143486
H	5.6299286561	0.388283505	0.9507747395
H	5.6299286561	0.388283505	0.9507747395

TS endo 0118

E(RB3LYP) = -706.412614792 A.U.

First frequency = -521.3151 cm^{-1}

H	-1.6544943468	-0.3323254005	-2.282372978
C	-1.1738017733	-0.829391957	-1.4475009297
H	-0.382802833	-1.5072798439	-1.7475645361
C	-1.8664444809	-1.0527758598	-0.2591826467

C	-1.1434755346	-1.6101224181	0.8194114462
C	0.1796668617	-2.0001550624	0.7231951186
H	0.7067709004	-2.313012593	1.6193556386
H	0.5679730549	-2.4198203413	-0.1968698198
C	1.3412744983	-0.1597064944	-0.0768808088
H	1.4558340659	0.1338799967	0.9637389942
C	2.5319260594	-0.8422721993	-0.7188047869
C	0.4329166507	0.5600018814	-0.8544054663
H	0.666306408	0.6689722105	-1.9131063929
C	-0.338337207	1.6975285992	-0.2286234893
C	-3.3233738651	-0.5947218847	-0.0351203981
H	-1.5880023477	-1.5721871337	1.8113156154
C	-4.1628559639	-1.8622780534	0.2588274244
C	-3.9186713352	0.0974404138	-1.2745063967
C	-3.4595175905	0.3773046605	1.1596449579
H	-2.9331719014	1.3157464399	0.9677921503
H	-3.063660573	-0.0478438401	2.0859338959
H	-4.5156223579	0.613427124	1.3326848531
H	-4.959122256	0.3770353169	-1.0790735623
H	-3.9101357516	-0.5602410221	-2.1493908059
H	-3.3735440758	1.0124793142	-1.5288526302
H	-5.2164467455	-1.6001110493	0.4109741966
H	-3.8087942603	-2.3748435065	1.1583879258
H	-4.1021074788	-2.5703170887	-0.574015201
H	-0.7202914381	1.3619155079	0.7434146952
H	-1.2153384534	1.9475872142	-0.8378835846
C	0.5092181833	2.964719333	-0.0241677675
H	1.378037002	2.7211640334	0.6019122224
C	-0.2799219232	4.1132217561	0.614404901
H	0.9155673132	3.2933127289	-0.9912707488
H	-0.6874598693	3.7772141979	1.5778513502
H	-1.1484725597	4.3493277836	-0.0156614208
C	0.5617590306	5.3751906987	0.8236266778
H	-0.0234574198	6.179545433	1.2813041058
H	0.9547600536	5.7485154988	-0.12901182
H	1.418803962	5.1727231765	1.4761406439
C	3.4519447402	-1.5888623917	0.2529772842
H	3.1306664533	-0.0859761332	-1.2492350943

H	2.1853892993	-1.5334372326	-1.5034384306
H	3.7704632682	-0.8976382491	1.0463565352
C	4.6896962244	-2.1842866136	-0.4265573986
H	2.8969666378	-2.3905347222	0.7545142471
C	5.6063115225	-2.9286659548	0.5483664903
H	5.2527304385	-1.381911876	-0.9225634521
H	4.3689144769	-2.8676854221	-1.2248203588
H	6.4823101342	-3.3447733803	0.0403282118
H	5.0764231156	-3.7569197269	1.0326674192
H	5.9651939288	-2.2603480128	1.339499336
H	5.9651939288	-2.2603480128	1.339499336

TS endo 0121

E(RB3LYP) = -706.414128257 A.U.

First frequency = -512.1437 cm⁻¹

H	-1.8403557012	0.1385441527	-1.9801621976
C	-1.4195179269	-0.631588174	-1.3442585238
H	-0.7533570148	-1.3082469348	-1.8655408857
C	-2.0852018717	-1.0545539014	-0.1975714229
C	-1.4196288999	-1.9776986271	0.6411862305
C	-0.1764185941	-2.5058099631	0.3396123114
H	0.3401735696	-3.1153984315	1.0760546818
H	0.0916918021	-2.7254982819	-0.6867142122
C	1.2131847768	-0.7425640695	0.0114307066
H	1.3733841083	-0.7230618172	1.0862845282
C	2.2755178253	-1.4403610129	-0.8107948024
C	0.4536997528	0.293159254	-0.5353716432
H	0.6801629863	0.5886098637	-1.5583008662
C	-0.1082446955	1.3659454465	0.3680090666
C	-3.4363760493	-0.4608577329	0.2553463535
H	-1.8089269708	-2.1367665832	1.6440501412
C	-3.3641026599	0.1624983318	1.668152063
C	-4.4620830951	-1.6205479544	0.2765443716
C	-3.9542401565	0.6214199891	-0.7090919497
H	-3.2724160371	1.4768102586	-0.760768672
H	-4.9244161254	0.9928268361	-0.3631529688
H	-4.0904486049	0.2303478696	-1.722235559

H	-4.1635365788	-2.4033145918	0.9804690314
H	-4.5508679231	-2.0788826442	-0.7137301715
H	-5.4512498174	-1.2548510804	0.5760302222
H	-3.0097797966	-0.5499334455	2.4179459488
H	-4.3589047225	0.4995345601	1.9808183828
H	-2.6971158155	1.0284324283	1.6837889156
H	-0.579626458	0.8748830769	1.2267701104
H	-0.9033500519	1.9168999096	-0.1460035324
C	0.9520218896	2.3568215679	0.8940986348
H	0.4487864109	3.1021322767	1.5261567182
C	1.7570144635	3.0815753205	-0.195377077
H	1.6473503252	1.8150829276	1.5477845794
H	2.3487115096	2.3468889974	-0.7554461221
H	2.4814852442	3.748505556	0.2888788872
C	0.8957206869	3.8913803574	-1.17042788
H	0.2696843546	4.6158728305	-0.6363451914
H	0.2284237941	3.2454683222	-1.7509279575
H	1.5161477895	4.4463880434	-1.8815424282
C	3.5536868323	-0.5989780721	-1.0181962928
H	1.863798684	-1.6845874232	-1.8002189927
H	2.5413481554	-2.3982130988	-0.3490102936
H	4.2703769356	-1.1906467143	-1.6050174343
C	4.2323689757	-0.1240185422	0.2756328663
H	3.3008055542	0.2776638858	-1.6279894701
C	4.6492700719	-1.2608376364	1.214687739
H	3.5583826003	0.5590726901	0.8065708866
H	5.1163070988	0.4686598405	0.0083899959
H	3.781030241	-1.8127460563	1.5900830829
H	5.1946058516	-0.8775038453	2.0831577678
H	5.2998077656	-1.9789903857	0.7017586929
H	5.2998077656	-1.9789903857	0.7017586929

TS endo 0126

E(RB3LYP) = -706.412712498 A.U.

First frequency = -516.0024 cm^{-1}

H	-1.1029700373	0.3807526315	-2.1823585306
C	-0.9579497355	-0.4195602182	-1.4671098163

H	-0.2911769831	-1.1984896458	-1.8128089805
C	-1.9069169332	-0.6929251804	-0.4898796029
C	-1.5981185428	-1.6819011187	0.4727455096
C	-0.4240414978	-2.4161810734	0.4446360906
H	-0.1979692107	-3.0896888645	1.267102748
H	0.0005597078	-2.7211143739	-0.5050444562
C	1.2582434196	-0.9854644836	0.5038091738
H	1.1686092889	-0.9191801541	1.586586133
C	2.3506046485	-1.907534456	0.0001937917
C	0.9229376462	0.158643645	-0.2217267645
H	1.4276868997	0.3064342693	-1.1756772507
C	0.4614656663	1.4122307995	0.487249225
C	-3.2294752411	0.0922078884	-0.3504087818
H	-2.2147241372	-1.7436679658	1.3659628518
C	-4.3846445888	-0.9153402632	-0.570198761
C	-3.3678141429	1.2100907302	-1.3990216576
C	-3.3869802345	0.7281564376	1.048870451
H	-3.3458631596	-0.0159213748	1.8487335273
H	-4.3544923588	1.2372908122	1.124937194
H	-2.6056304345	1.4680363737	1.236440267
H	-2.5899320974	1.970668465	-1.2857464316
H	-4.3356195858	1.7090663576	-1.2831836654
H	-3.3173948662	0.8172104928	-2.4192714179
H	-4.3609082599	-1.7178599118	0.1731507649
H	-4.314821794	-1.3761984193	-1.5608532922
H	-5.3548976992	-0.4106738622	-0.4935972263
H	1.1910290248	1.6616553371	1.2739333741
H	-0.4761904948	1.1971090909	1.0142229998
C	0.3143816248	2.6283981554	-0.4343112112
H	1.2285659792	2.7179024176	-1.037143912
C	0.0799132058	3.9587012138	0.2961909248
H	-0.4997584847	2.451467642	-1.1468427511
H	0.0828415231	4.7701365523	-0.4427804137
H	0.9284294731	4.1547706825	0.9661350121
C	-1.2238388501	4.0189019353	1.0992504521
H	-2.0898769676	3.8069410759	0.4620445826
H	-1.3705966103	5.0093174928	1.542523446
H	-1.228527748	3.2906080396	1.9164307698

C	3.7617916552	-1.3569495783	0.2688394579
H	2.2282641871	-2.0596840442	-1.0821852107
H	2.2636617731	-2.8998329794	0.4612484546
H	3.8621202089	-0.3768920531	-0.2165199692
C	4.8776283389	-2.2895969226	-0.2151593891
H	3.8792537083	-1.1745198706	1.3463803937
C	6.2790430617	-1.7330970848	0.0522778681
H	4.7529961638	-2.4731481622	-1.2912339198
H	4.7696873382	-3.2675368387	0.2736042303
H	6.4229127909	-0.7703750146	-0.4514202646
H	7.0584482041	-2.4152643155	-0.3027066149
H	6.4400660121	-1.5707421678	1.1241807756
H	6.4400660121	-1.5707421678	1.1241807756

TS endo 0134

E(RB3LYP) = -706.412407467 A.U.

First frequency = -493.2291 cm⁻¹

H	-1.4809239306	-0.7934407208	-2.1298867029
C	-1.1690198157	-1.1844310385	-1.1662633704
H	-0.40107825	-1.943904169	-1.2306268519
C	-2.025893171	-1.1315813116	-0.0728829816
C	-1.5219842816	-1.5544593395	1.1796535326
C	-0.2508629995	-2.0781018072	1.337221746
H	0.1234865797	-2.2827601196	2.3364320136
H	0.1929715123	-2.690234364	0.5609450096
C	1.1930572499	-0.5170631339	0.5747015668
H	1.1287511156	-0.0346667382	1.5477095195
C	2.4044523387	-1.3971298533	0.3593243732
C	0.5923061071	0.1396420912	-0.4968568088
H	1.0139303851	-0.027235363	-1.4868557661
C	-0.1034819468	1.4600329313	-0.2784343677
C	-3.4502046143	-0.5501670272	-0.2189874614
H	-2.0694730515	-1.2911074549	2.0786253967
C	-4.1354800161	-0.3077260938	1.1392821843
C	-4.2876831171	-1.5903752392	-1.003518468
C	-3.4681907322	0.7841863169	-0.9951892896
H	-2.9555441043	1.5725418437	-0.4387230413

H	-4.5030524459	1.1050551162	-1.1583298836
H	-2.9953503646	0.7011837817	-1.9775150741
H	-4.3001747408	-2.5529232043	-0.4818097502
H	-3.8698621198	-1.7566460986	-2.001218222
H	-5.3233430276	-1.248968936	-1.1184127209
H	-4.2413769455	-1.2326166381	1.7146970934
H	-5.1408863541	0.0950682415	0.9788781122
H	-3.5811094011	0.4144069516	1.748028125
H	-0.7892669475	1.357883791	0.5740703148
H	-0.7211294201	1.7125984809	-1.1464727886
C	0.871673674	2.6187664338	-0.0025958877
H	1.4847364157	2.3757073254	0.8754557217
C	0.1600281428	3.9577800663	0.2203206808
H	1.5734492633	2.7122517966	-0.8434439044
H	-0.5442319594	3.8555145629	1.0575137015
H	-0.4508318456	4.1942881156	-0.6616775845
C	1.127854191	5.1110152181	0.500040706
H	0.5963434775	6.0554076574	0.656897311
H	1.8223235984	5.2534408297	-0.3358767706
H	1.7278203013	4.9125712855	1.3955810393
C	3.7027843124	-0.5769231618	0.2353982586
H	2.2565815606	-1.993044631	-0.5511075297
H	2.5171261669	-2.1139676236	1.1833204353
H	3.6129694663	0.1014770802	-0.6237621481
C	4.9750908436	-1.4261510206	0.0936360186
H	3.7946928716	0.0660811172	1.1208239999
C	5.0325235115	-2.254214984	-1.1953157865
H	5.0626927626	-2.0935007816	0.9621452772
H	5.847770616	-0.761708572	0.1314519405
H	5.9847789447	-2.7875264906	-1.2818479415
H	4.9281288929	-1.6119826639	-2.077761868
H	4.2337505639	-3.0017544724	-1.2346914991
H	4.2337505639	-3.0017544724	-1.2346914991

TS endo 0136

E(RB3LYP) = -706.413772881 A.U.

First frequency = -525.5812 cm^{-1}

H	-1.1218156694	0.0172274577	-2.0901184305
C	-0.9934736493	-0.7288563679	-1.3151057296
H	-0.3976576202	-1.5774677537	-1.623668709
C	-1.913293439	-0.8541238572	-0.2800760507
C	-1.6196937571	-1.773118811	0.7525430405
C	-0.5096893348	-2.6049665139	0.7176684765
H	-0.2834901313	-3.2256932859	1.5807816002
H	-0.1958148871	-3.0351841531	-0.2270249032
C	1.2898885156	-1.3656224812	0.5375922156
H	1.3167185357	-1.2698769812	1.6220240831
C	2.2568043832	-2.3831854022	-0.0347410744
C	0.9624468617	-0.2081913494	-0.1746241673
H	1.4020917819	-0.0738343943	-1.1602489565
C	0.5952537431	1.0435813211	0.5838630371
C	-3.1655692003	0.0415907197	-0.1499692992
H	-2.17848274	-1.7028443289	1.6830393756
C	-3.3885770124	0.9277299024	-1.3895668754
C	-3.0936613046	0.9576676898	1.0916198755
C	-4.3958283714	-0.8889448941	-0.014347716
H	-4.3351243797	-1.5144636182	0.8806724868
H	-4.4773909955	-1.5536194897	-0.8803928272
H	-5.3161435897	-0.2972554787	0.051816959
H	-2.9265817185	0.3886605985	2.0105741469
H	-4.0312391663	1.5129597077	1.209760645
H	-2.2847230687	1.6857887085	0.9942939371
H	-3.4653085358	0.3285233095	-2.302275973
H	-2.5837119056	1.6559610995	-1.5265145142
H	-4.3207938357	1.4914767404	-1.2784229829
H	1.4297919319	1.304036946	1.254133013
H	-0.2489438239	0.8137806452	1.2487031347
C	0.2747257636	2.2591131194	-0.2866301908
H	1.1030688293	2.4302990927	-0.9890370047
C	0.0275433938	3.5385804187	0.5193167903
H	-0.6033625886	2.0412453224	-0.9041361652
H	0.9281470608	3.7814247946	1.0994184011
H	-0.7653163272	3.3576498256	1.2576430485
C	-0.35814541	4.7301542524	-0.3613232562
H	-1.2796081376	4.5235481299	-0.9179299897

H	0.4268456541	4.9491419448	-1.0942681674
H	-0.5227241152	5.6352136211	0.2323137385
C	3.7370986302	-2.0650023771	0.2628427233
H	2.1129788459	-2.4472653099	-1.1230218296
H	2.0400441547	-3.3822618229	0.3633767811
H	3.8768856068	-2.0062188766	1.3517276743
C	4.268156564	-0.780080246	-0.3818688901
H	4.3492165179	-2.912630507	-0.0757255971
C	5.756153857	-0.5509281136	-0.101273925
H	3.6891032198	0.0773073424	-0.0199497036
H	4.0987806621	-0.8243861821	-1.46687079
H	6.1160184489	0.3719272904	-0.5678489582
H	6.3643844821	-1.3782441348	-0.484790078
H	5.9458080947	-0.4755412762	0.9757256031
H	5.9458080947	-0.4755412762	0.9757256031

TS endo 0137

E(RB3LYP) = -706.411876658 A.U.

First frequency = -523.2880 cm^{-1}

H	-1.8514605212	-0.4932172569	-2.2366807152
C	-1.3313920509	-0.9133229424	-1.3832281993
H	-0.4920658363	-1.5423274619	-1.6576880955
C	-2.0023831905	-1.1383647575	-0.1823723773
C	-1.2361517197	-1.5905533537	0.9145098859
C	0.1148770897	-1.8727606191	0.8290099186
H	0.6661015251	-2.1025084647	1.7357276841
H	0.5363530024	-2.2987814028	-0.0734434668
C	1.1082921183	0.0224290766	-0.0467243105
H	1.182681786	0.3770084786	0.9772589855
C	2.3642428874	-0.5827142262	-0.6422515502
C	0.1585378312	0.626946689	-0.8738023828
H	0.4006695345	0.6815127162	-1.9355286543
C	-0.6979250497	1.7599801438	-0.3538013214
C	-3.4877673175	-0.7798092244	0.0337856943
H	-1.6805893123	-1.5457868931	1.9062149311
C	-4.1453107521	-0.2081290192	-1.2352192184
C	-3.6806662788	0.247816414	1.1727971347

C	-4.2286946157	-2.0858054494	0.4117541243
H	-4.125586673	-2.8342777208	-0.3805776702
H	-5.2968718306	-1.8921152548	0.5646332972
H	-3.8290373996	-2.5191910456	1.3334605556
H	-3.2152379667	1.2048261507	0.9237689863
H	-3.2526467409	-0.0985213904	2.1174354985
H	-4.748698632	0.4260359093	1.3421941197
H	-3.67846504	0.7319219219	-1.5473506172
H	-5.2035433876	-0.0021205725	-1.0438824916
H	-4.0892579498	-0.9115110742	-2.072022614
H	-0.9622088588	1.5502432036	0.6901671458
H	-1.6411284298	1.8044556492	-0.9092688839
C	-0.0229349812	3.1451156184	-0.4426979752
H	0.2431820947	3.3485930373	-1.4899571097
C	1.2203537532	3.3263346933	0.4351956615
H	-0.7652418182	3.9072719388	-0.1665622391
H	1.9901595541	2.6063898345	0.1347041909
H	0.9654568075	3.0812562527	1.4757126897
C	1.7898237312	4.7463053692	0.364511898
H	1.0524457027	5.4863681124	0.6963368163
H	2.0752635038	5.0046605888	-0.6618712169
H	2.6787584261	4.8554359908	0.9944872336
C	3.3357538546	-1.1907665374	0.3747566295
H	2.8998669905	0.1967524866	-1.2057904343
H	2.0923430558	-1.3410714511	-1.3933964236
H	3.5759280982	-0.4342859101	1.1355404461
C	4.6339593296	-1.6982527521	-0.2619982556
H	2.851900206	-2.0161683352	0.9101396121
C	5.6026887401	-2.3031591664	0.7580133897
H	5.1257110181	-0.8711806605	-0.7920880672
H	4.3908508779	-2.4473696353	-1.028070463
H	5.146604956	-3.1532893621	1.2781974929
H	5.8851391482	-1.5655615861	1.5179461696
H	6.5214104004	-2.6583922036	0.280126129
H	6.5214104004	-2.6583922036	0.280126129

TS endo 0142

E(RB3LYP) = -706.412275408 A.U.

First frequency = $-527.8386 \text{ cm}^{-1}$

H	-0.9612192414	-0.7360853713	-2.0552493487
C	-0.7295985224	-1.0817327666	-1.0545198659
H	0.1054897097	-1.7678062147	-1.0146428874
C	-1.7077869211	-1.1165191828	-0.0648965246
C	-1.3009863495	-1.4606501865	1.2436636356
C	0.0064342737	-1.7878479918	1.5623632545
H	0.2848158398	-1.9220567939	2.6041777211
H	0.6167003715	-2.348335432	0.8645679898
C	1.2903522375	-0.0629145164	0.9002445134
H	1.0120813774	0.4484655795	1.8192516555
C	2.6549210097	-0.7298720285	0.9566822748
C	0.7296406557	0.4450656566	-0.2746516418
H	1.2858653885	0.3300562146	-1.2015926569
C	-0.1627551819	1.6615796658	-0.1932540925
C	-3.1638168738	-0.6627250776	-0.306463212
H	-1.9903242676	-1.2736727947	2.0637699416
C	-3.582227693	0.4983055997	0.6247277414
C	-4.0773107105	-1.8803853137	-0.0236028593
C	-3.4040121047	-0.2102738013	-1.7580393065
H	-2.7935808546	0.6612478847	-2.0167104233
H	-4.4538367143	0.0716878941	-1.8896959402
H	-3.1818047587	-1.0083535311	-2.4733607947
H	-3.979415276	-2.2206664629	1.0117271285
H	-3.8183117463	-2.7202235926	-0.6764418944
H	-5.1285007454	-1.6217938815	-0.1968677471
H	-3.0041893611	1.4016530297	0.4131971146
H	-3.4467038417	0.2509416104	1.6810521304
H	-4.6419128054	0.7355304623	0.4766529936
H	-0.850706851	1.5317044246	0.6510290201
H	-0.7856153821	1.7453270549	-1.092060672
C	0.6205425488	2.9717837526	-0.0015116707
H	1.2310645018	2.8975685475	0.9085665254
C	-0.2882286247	4.203000691	0.0873312485
H	1.3293669205	3.0990604819	-0.8320494111
H	-0.9963796169	4.0678883777	0.9165057391
H	-0.8983849466	4.2684560081	-0.8239790819

C	0.4880860125	5.5085870053	0.281214909
H	1.0814189044	5.4804455214	1.2023397463
H	-0.1826175834	6.3719344372	0.3425604709
H	1.1804065418	5.681952755	-0.5506469934
C	3.0769314516	-1.5272880336	-0.2840051669
H	2.7054793974	-1.3900299234	1.8329214752
H	3.410227673	0.0509027872	1.1384258564
H	2.3242731668	-2.29323044	-0.5148618516
C	4.441367007	-2.2057871133	-0.1165387039
H	3.1137669427	-0.8662508594	-1.1593464348
C	4.8736344998	-2.9904953752	-1.3582651646
H	4.4066400219	-2.8782424462	0.7512894819
H	5.1963223364	-1.4436456922	0.1200023757
H	5.8490091314	-3.4664245276	-1.2145346614
H	4.9478592818	-2.3343339568	-2.2330377128
H	4.1500122267	-3.778046193	-1.598072394
H	4.1500122267	-3.778046193	-1.598072394

TS endo 0146

E(RB3LYP) = -706.413690660 A.U.

First frequency = -524.9626 cm^{-1}

H	-1.3865036278	0.0364264961	-2.0871412901
C	-1.1368988794	-0.6932922837	-1.326146631
H	-0.5503840906	-1.5238888439	-1.6965167996
C	-1.9195111329	-0.8372404045	-0.1864163761
C	-1.4702152239	-1.7312892882	0.8120600855
C	-0.347778468	-2.5303370766	0.652086976
H	0.0022818877	-3.1279529134	1.4897088571
H	-0.1351623541	-2.9653581028	-0.3180510256
C	1.3730673758	-1.2249892841	0.2242625534
H	1.5314235381	-1.1281225953	1.2954091909
C	2.2688263089	-2.2175907718	-0.490870339
C	0.922689287	-0.0833502077	-0.4412750935
H	1.2316827829	0.0604191099	-1.4752001719
C	0.6083610385	1.1603340931	0.3530127907
C	-3.1793659875	0.0148052085	0.0860522884
H	-1.913667662	-1.6646121407	1.8030417647

C	-2.9913281125	0.9508719249	1.3003012269
C	-4.348722852	-0.9567956676	0.3802528889
C	-3.5842033447	0.8738340562	-1.1263175572
H	-4.5163370029	1.4055363046	-0.9081468295
H	-3.7489860593	0.2585297512	-2.016389893
H	-2.8297516401	1.62820868	-1.3684562158
H	-4.5102657872	-1.6366139716	-0.4625015435
H	-5.2754600151	-0.3972771175	0.552158943
H	-4.1565764082	-1.5665819758	1.2675408313
H	-2.2269757114	1.7051817846	1.0986741788
H	-2.694163582	0.4013101666	2.197997
H	-3.9273415744	1.4747710421	1.5256003643
H	1.511689416	1.4586748601	0.9082595561
H	-0.1338032027	0.9043620241	1.1220483582
C	0.1292225549	2.3540998818	-0.4737746117
H	0.851289314	2.5509528293	-1.2791651851
C	-0.0623005888	3.6308433752	0.3514109243
H	-0.8122725304	2.0955929825	-0.970407611
H	0.895973081	3.9155641812	0.8066056336
H	-0.743141087	3.4259396959	1.1886434941
C	-0.6091526619	4.7966807396	-0.4768299068
H	-1.5865670332	4.5473563981	-0.9059011383
H	0.0628605784	5.039146659	-1.3080835172
H	-0.7312553829	5.7006681721	0.1285759562
C	3.7144111162	-1.7182252515	-0.6845248428
H	1.8401272747	-2.4394752402	-1.4784016564
H	2.2920736825	-3.1692412433	0.0557559594
H	4.2713526459	-2.4608789103	-1.2730592085
C	4.4645088685	-1.4545330275	0.6262754292
H	3.6978188195	-0.7969994384	-1.2823789791
C	5.9133328546	-1.0130142879	0.401271732
H	4.4462111552	-2.3646237464	1.2420532996
H	3.9334760517	-0.6858614716	1.2014121978
H	5.9553531162	-0.0896771746	-0.1879018604
H	6.4791216624	-1.7770755714	-0.1442220123
H	6.4302550985	-0.8276553968	1.3485279442
H	6.4302550985	-0.8276553968	1.3485279442

TS endo 0154

E(RB3LYP) = -706.412096069 A.U.

First frequency = -520.8418 cm^{-1}

H	-1.9210243463	-0.3268279068	-2.258128272
C	-1.3760878802	-0.8737589999	-1.4971446635
H	-0.6785310207	-1.5972067961	-1.9038625238
C	-1.9310772096	-1.0782157977	-0.235097733
C	-1.1212544813	-1.7077553105	0.736842783
C	0.1489044463	-2.1854154804	0.4710196505
H	0.7594446902	-2.5533301323	1.290138374
H	0.3906604395	-2.609263876	-0.4958721936
C	1.3273067791	-0.4068403215	-0.4455576902
H	1.580215612	-0.1461568093	0.5775601609
C	2.3736194782	-1.1549298688	-1.2481366135
C	0.3810651066	0.3899890665	-1.0915374927
H	0.4894191622	0.5108828534	-2.1690731281
C	-0.2242483101	1.5607549745	-0.3543377339
C	-3.3142613334	-0.529326495	0.1749892836
H	-1.4362959734	-1.6624729059	1.7768847875
C	-4.1976052438	-1.7447376276	0.5495647507
C	-4.0069290022	0.2318670123	-0.9697086368
C	-3.2357731741	0.4196890189	1.393198573
H	-2.6732080529	1.3254795305	1.15320991
H	-2.7600967728	-0.0537406098	2.256318934
H	-4.2439418439	0.7212495223	1.6993480647
H	-4.9934383345	0.5762085239	-0.6423944657
H	-4.1517906081	-0.40302321	-1.849454604
H	-3.434153273	1.1139370358	-1.2746665991
H	-4.2883225705	-2.4343950908	-0.2958768133
H	-5.2039589729	-1.4164900663	0.8349313893
H	-3.7727836104	-2.3020307738	1.3899604823
H	-0.5110407965	1.2248642453	0.649812424
H	-1.1468044877	1.8902487761	-0.8475513772
C	0.7337585809	2.7575205385	-0.2277768301
H	1.651231965	2.4332506306	0.2814277176
C	0.1155506515	3.9391011848	0.5279643384
H	1.0439034068	3.085904578	-1.2299376064

H	-0.1970494954	3.6031867537	1.5263030634
H	-0.8023618709	4.2565694147	0.0143905442
C	1.0686695435	5.1301953803	0.6608167785
H	1.9803552855	4.846332711	1.1989206995
H	0.6048743333	5.9598185717	1.204468553
H	1.3711501971	5.5039133349	-0.324159269
C	3.3622424774	-2.0053552134	-0.4366092815
H	2.9527298867	-0.4280554975	-1.8383815719
H	1.870039415	-1.7906195753	-1.992169843
H	2.8195583614	-2.7566016746	0.1496652628
C	4.2665965086	-1.1916049671	0.4983771341
H	3.9965807862	-2.5666908433	-1.1356467348
C	5.2734124128	-2.0647671131	1.252800252
H	3.6550676665	-0.6380571678	1.2217208897
H	4.8012103033	-0.4330893035	-0.0897817321
H	5.9110298697	-1.4671615265	1.9123299241
H	5.925546972	-2.6055164761	0.5573108193
H	4.7610528022	-2.8113124274	1.8705949258
H	4.7610528022	-2.8113124274	1.8705949258

TS endo 0161

E(RB3LYP) = -706.412962338 A.U.

First frequency = -507.7715 cm^{-1}

H	-1.703521009	-0.2341089882	-2.1396464725
C	-1.406668009	-0.915359038	-1.3477595188
H	-0.6992396288	-1.6699144772	-1.6649418644
C	-2.2514709537	-1.1448874828	-0.2651414621
C	-1.7622894479	-1.9469421361	0.7902798775
C	-0.5229487861	-2.5632975469	0.742891659
H	-0.1471001067	-3.078607435	1.6225906779
H	-0.1422444014	-2.9493331845	-0.1953869593
C	1.0193339247	-0.9612458559	0.4284985202
H	1.0066463122	-0.7882074244	1.5033154749
C	2.1632498446	-1.824817273	-0.0660620034
C	0.437643386	0.0263127045	-0.3699856379
H	0.8257710739	0.1508868032	-1.3781081475
C	-0.1833398927	1.2418788653	0.2817228233

C	-3.6410895043	-0.472661894	-0.1958977571
H	-2.281196639	-1.9335944604	1.7430339197
C	-4.5359202529	-1.1711098124	-1.24987957
C	-3.5875709002	1.0361709132	-0.5167456589
C	-4.3099992839	-0.6328405838	1.182447442
H	-5.2940722819	-0.1529100985	1.1732333781
H	-3.7187562189	-0.1633185428	1.9757140238
H	-4.4608580723	-1.6849738449	1.4432439829
H	-4.6037158229	1.4440460102	-0.5568602804
H	-3.1171365476	1.2398794378	-1.482516772
H	-3.0358379393	1.5837945804	0.2512898841
H	-4.1309570286	-1.0379814765	-2.2577791753
H	-5.5516530562	-0.7584766751	-1.2318611513
H	-4.5995597164	-2.2465818544	-1.0546861754
H	-0.8158125527	0.8949977467	1.1091152101
H	-0.8457549906	1.7533927239	-0.4233647027
C	0.8483893395	2.2568273053	0.8159147595
H	0.3462657337	2.9665880706	1.4878422088
C	1.5559469295	3.0466193671	-0.2932782792
H	1.592047942	1.728508236	1.4275786239
H	0.8151701462	3.6682872208	-0.8141725559
H	1.9496836726	2.3537582105	-1.0470689036
C	2.695489125	3.9230101467	0.232443968
H	3.1636470899	4.5021175779	-0.5702769629
H	3.4748829407	3.3097345967	0.6995939233
H	2.3348630503	4.6298441916	0.988658171
C	3.5601329698	-1.2669573536	0.2794421961
H	2.0810315597	-1.9476428857	-1.1554526925
H	2.0945027107	-2.8324966275	0.3618985501
H	3.6287331565	-1.1318467738	1.3684703718
C	3.9165551422	0.0507057649	-0.4135638831
H	4.3124017332	-2.0249006014	0.0201627972
C	5.3156593123	0.5569002599	-0.0528130616
H	3.1760603102	0.8086130866	-0.1448519753
H	3.837914619	-0.0803346388	-1.5019320434
H	6.0881990359	-0.1661766081	-0.3389024421
H	5.4055658967	0.7240594802	1.0269285629
H	5.5406908068	1.5034268548	-0.5552792065

H 5.5406908068 1.5034268548 -0.5552792065

TS endo 0171

E(RB3LYP) = -706.411803250 A.U.

First frequency = -524.5903 cm⁻¹

H -2.1012359538 -0.222829167 -2.241316508
C -1.5282601219 -0.7928635095 -1.5187282601
H -0.7885273343 -1.4425164222 -1.9732934793
C -2.0803933158 -1.130853455 -0.2834422293
C -1.2426951571 -1.786940854 0.6452708054
C 0.0585289762 -2.1586832067 0.3606963166
H 0.683426327 -2.5526298894 1.1566142648
H 0.3370284952 -2.4870735619 -0.6329242815
C 1.1142325588 -0.2383430625 -0.390869195
H 1.3200869805 -0.0393579572 0.6552534027
C 2.2324210051 -0.8595249725 -1.2062585402
C 0.1365482115 0.543362989 -1.0106606762
H 0.2657126467 0.7310651067 -2.0770309501
C -0.5450820717 1.6547268258 -0.2437028168
C -3.494102666 -0.6942061089 0.1556527118
H -1.5696825908 -1.8456689434 1.6809999221
C -4.3048432618 -1.9799784745 0.4506532072
C -4.2327629698 0.0948531549 -0.9403135753
C -3.4659606978 0.1784346946 1.431703229
H -2.9695769974 -0.3258672956 2.2652306716
H -4.4881403392 0.4115989136 1.75100327
H -2.9459177748 1.1228258213 1.2523409232
H -4.3345182107 -0.4890850405 -1.8605165094
H -3.7187737156 1.0304003356 -1.1843955242
H -5.2398744728 0.3527460863 -0.5966536792
H -5.3275765754 -1.7288796227 0.755397523
H -3.8474244607 -2.5650870646 1.254104934
H -4.3582659407 -2.6179968943 -0.4374425809
H -0.7217824822 1.3143822082 0.7842128419
H -1.5304430242 1.8619247408 -0.6756381634
C 0.2550185385 2.9743654096 -0.2143906738
H 0.4325872017 3.3103629922 -1.2461340495

C	1.5935693185	2.9147607872	0.5308772736
H	-0.3741350187	3.7466267315	0.2503152017
H	2.2549928385	2.189845559	0.0432502721
H	1.4232323011	2.5333720235	1.5474995573
C	2.2900203878	4.2768811953	0.6016122417
H	3.2455513082	4.2126931751	1.132476073
H	1.6678279424	5.0145947782	1.1213910711
H	2.4925734047	4.6673007087	-0.4024977305
C	3.3178339777	-1.5685985566	-0.3838176715
H	2.7150267285	-0.0758229304	-1.8097890501
H	1.8069816242	-1.5618270002	-1.9391180986
H	2.8603047898	-2.3370560996	0.2517007188
C	4.1500875066	-0.6184324856	0.4880387588
H	3.9930949683	-2.1002295756	-1.0672078182
C	5.2349895346	-1.3450141186	1.2878453396
H	3.4941811831	-0.0727691626	1.1778023773
H	4.611629187	0.143833368	-0.1548640774
H	5.9287272873	-1.8725571301	0.6231252799
H	4.794712678	-2.0895230638	1.9611141447
H	5.8205994157	-0.6492283302	1.8974312187
H	5.8205994157	-0.6492283302	1.8974312187

TS endo 0172

E(RB3LYP) = -706.413011166 A.U.

First frequency = -526.1468 cm^{-1}

H	-1.2106275102	0.5859224954	-1.8861847112
C	-1.0202748851	-0.3031260467	-1.2969950926
H	-0.2647172928	-0.951612155	-1.7204618699
C	-1.983250536	-0.8121710695	-0.4338851705
C	-1.6211074493	-1.9077184235	0.3823982217
C	-0.3894535158	-2.5408601075	0.2812928649
H	-0.1342698208	-3.3192687156	0.9957571547
H	0.0585796634	-2.6794250209	-0.6966231296
C	1.1906337598	-1.0587045993	0.590437
H	1.1481009165	-1.2563689303	1.6600152786
C	2.3346200691	-1.7260570747	-0.1439598219
C	0.7222635836	0.1888676648	0.1724988242

H	1.196198881	0.6474471776	-0.6916841017
C	0.061735798	1.0969892751	1.1797831082
C	-3.3731627635	-0.1639067393	-0.2439729926
H	-2.254211503	-2.1515416823	1.2325183394
C	-4.4377834336	-1.2624808825	-0.4842691967
C	-3.6376207003	0.968938435	-1.2530972556
C	-3.5587248718	0.4065803884	1.1800696154
H	-3.3722145635	-0.3476108334	1.9499048966
H	-4.5847609625	0.7688219161	1.3120888002
H	-2.8828652319	1.2468979835	1.3594042527
H	-2.9550441809	1.8123793917	-1.1134836337
H	-4.6558855441	1.3501376087	-1.1225542419
H	-3.5408863326	0.6175659622	-2.2851980848
H	-4.3355989173	-1.6895679538	-1.4871063377
H	-5.4464594828	-0.8437193388	-0.3909963456
H	-4.3467742683	-2.0801258433	0.236412405
H	0.7587398837	1.2659313338	2.0156239722
H	-0.7856012918	0.5507359098	1.615503568
C	-0.3978849418	2.4582059602	0.6477253385
H	-1.0622241171	2.3064133226	-0.2103368608
C	0.7491806987	3.3907688147	0.2368582403
H	-0.9996207688	2.9601228097	1.417518211
H	1.3615184093	2.9092423647	-0.5361576716
H	1.4142343238	3.5440388714	1.0977152404
C	0.2527697239	4.7436143316	-0.2810424422
H	-0.3360674766	5.2655106613	0.4820775555
H	-0.3891469239	4.6159334101	-1.1603854242
H	1.0836603936	5.39699183	-0.5664499825
C	3.7029581441	-1.1163197151	0.2061883273
H	2.1724390311	-1.637970781	-1.228372838
H	2.3578400454	-2.8012980838	0.0761427176
H	3.6907121917	-0.0453908374	-0.0368026095
C	4.8717638316	-1.796038579	-0.5155230917
H	3.8581498011	-1.1780398604	1.292547202
C	6.2292560553	-1.1802662242	-0.1644937447
H	4.7094204342	-1.7367418557	-1.6005457215
H	4.8770887855	-2.8663324058	-0.2678640083
H	6.4292418575	-1.2553064941	0.9105118337

H	6.260186017	-0.1176851452	-0.4313402195
H	7.0477921966	-1.6808546159	-0.6919552113
H	7.0477921966	-1.6808546159	-0.6919552113

TS endo 0186

E(RB3LYP) = -706.411572498 A.U.

First frequency = -529.0083 cm⁻¹

H	-1.1211665907	-0.704282021	-2.1379211992
C	-0.8638040674	-1.0477598579	-1.1426954654
H	0.0237649099	-1.6653763153	-1.1128991084
C	-1.838411544	-1.1831438214	-0.1578639566
C	-1.4074473744	-1.5190792593	1.1444198609
C	-0.0769361835	-1.7356366958	1.4613190838
H	0.2101682467	-1.8652921316	2.5013528854
H	0.5815819811	-2.2270364935	0.7552093689
C	1.0373402492	0.1113525324	0.840738209
H	0.6968194932	0.5876049413	1.7565060323
C	2.4570453958	-0.4278566615	0.9206173259
C	0.4627774645	0.5829333773	-0.3443524736
H	1.0471211132	0.5042647455	-1.2585320102
C	-0.5027664256	1.7479570327	-0.3072960262
C	-3.3243850358	-0.8358910444	-0.390825904
H	-2.1116181079	-1.4068405784	1.9655974667
C	-3.606369017	-0.4067133643	-1.8419339552
C	-3.8101146216	0.2971768348	0.5420099909
C	-4.1509515313	-2.1117734069	-0.0984624858
H	-4.022198559	-2.4441272216	0.9359477454
H	-3.8423633186	-2.9331133298	-0.7532996464
H	-5.2185854553	-1.9243529055	-0.2623247216
H	-4.8825116421	0.4713659831	0.3974427439
H	-3.2860040335	1.232724928	0.3301506628
H	-3.6559756188	0.0566987817	1.5974524106
H	-3.3249806331	-1.1868472142	-2.5563138484
H	-3.0682343256	0.5094478738	-2.1065902477
H	-4.6756718078	-0.2081526692	-1.9689149015
H	-1.1113436056	1.674490028	0.6024196692
H	-1.1989212062	1.6936235074	-1.1514892131

C	0.1901410424	3.1268982361	-0.3457487426
H	0.7976864921	3.1978163215	-1.2594635587
C	1.0695370936	3.450050422	0.8672619852
H	-0.5855196307	3.9002667112	-0.4381410668
H	1.8784941199	2.7140600392	0.9398764177
H	0.4742880919	3.3382664611	1.7841838102
C	1.6632231805	4.8604987713	0.8064582062
H	2.2833155282	4.9877066832	-0.0885339618
H	2.2906688578	5.0714387334	1.6787122203
H	0.8748797897	5.6212481194	0.7703782645
C	2.978199112	-1.1673163114	-0.318066881
H	2.5507744765	-1.090024202	1.7915343567
H	3.1330726764	0.4173884322	1.1264122278
H	2.2994143193	-1.9901836076	-0.580133384
C	4.3904407201	-1.7302536862	-0.1213748405
H	2.9820834096	-0.4918194566	-1.1830771516
C	4.9220187289	-2.454528539	-1.3612421482
H	4.3894653068	-2.41760922	0.7353793293
H	5.0708030774	-0.9107963794	0.1476864369
H	4.9642670229	-1.7798694764	-2.2239848001
H	4.2749357271	-3.2963878405	-1.6331225531
H	5.9300101052	-2.8485116443	-1.1961723379
H	5.9300101052	-2.8485116443	-1.1961723379

TS endo 0190

E(RB3LYP) = -706.412137437 A.U.

First frequency = -506.8453 cm⁻¹

H	-2.0614704712	-0.7254844043	-2.1451407328
C	-1.6119007656	-1.1854177119	-1.2701469426
H	-0.9066754321	-1.9718399615	-1.5048323274
C	-2.2787923952	-1.1737827648	-0.0482931469
C	-1.5955280006	-1.6873682813	1.0766647479
C	-0.3349243308	-2.2531673791	0.9886064771
H	0.1924002497	-2.5286355805	1.8978408666
H	-0.0559079343	-2.836464145	0.118942075
C	1.0148415639	-0.7009413537	0.0884145155
H	1.1103177043	-0.2659192159	1.0788572436

C	2.1366370438	-1.620750796	-0.3570756468
C	0.291320727	0.0279662176	-0.8580147702
H	0.5538717749	-0.1287032555	-1.9042863107
C	-0.2979070452	1.3837069639	-0.5424435715
C	-3.6854925006	-0.5461473289	0.0744803924
H	-1.9767861534	-1.4641256144	2.0676238838
C	-4.1433254297	-0.397909765	1.53798417
C	-4.6739225229	-1.4966147279	-0.645606536
C	-3.771339735	0.8466769239	-0.5846630399
H	-4.803786789	1.2119962825	-0.5502678238
H	-3.4683384393	0.8287051031	-1.6351728238
H	-3.1405841454	1.5700976578	-0.0618501517
H	-4.4222346808	-1.5934913568	-1.7062020695
H	-5.7006169931	-1.118946299	-0.5707855516
H	-4.6439190092	-2.4973163239	-0.2023532938
H	-3.4792105421	0.2635813975	2.1042743521
H	-4.18701867	-1.3630603814	2.0521317227
H	-5.1483749019	0.0354174845	1.5681253807
H	-0.7113867299	1.3666416788	0.4750058733
H	-1.1364565264	1.5833390814	-1.2143902367
C	0.6978928105	2.5576273024	-0.6755364028
H	1.1374345424	2.5401029259	-1.6833143072
C	1.8234525915	2.5893037998	0.3619571473
H	0.1297759717	3.4964370719	-0.6108967037
H	2.4156754186	1.67420802	0.2820950627
H	1.3862145257	2.5843148257	1.3702363819
C	2.7455040475	3.8015210533	0.2033125108
H	2.1916437021	4.7413438906	0.3103936245
H	3.2162196157	3.8086366083	-0.7868220087
H	3.545367951	3.7973601706	0.9512268632
C	3.4770030665	-0.8905090604	-0.5822219413
H	1.8345665017	-2.1101170239	-1.2930528446
H	2.2975691499	-2.4255265955	0.3719392615
H	4.1598192126	-1.5471802842	-1.1387484365
C	4.1671528549	-0.4558342488	0.7176135332
H	3.3028130264	-0.0144193313	-1.2212615363
C	5.4032321885	0.4128705285	0.4708325563
H	4.4465153294	-1.3517169112	1.288424107

H	3.4597608673	0.0947762737	1.3495175272
H	5.899876381	0.6840883433	1.4081142195
H	5.1295468804	1.3417602626	-0.0428999414
H	6.1349315662	-0.1083885516	-0.1571740016
H	6.1349315662	-0.1083885516	-0.1571740016

TS endo 0200

E(RB3LYP) = -706.413165803 A.U.

First frequency = -523.9804 cm^{-1}

H	-0.9757168594	-0.0050130922	-2.0267090941
C	-0.8021198688	-0.6633684249	-1.1839658685
H	-0.0800779602	-1.4439736008	-1.3838383513
C	-1.7617767563	-0.8290520831	-0.1924996309
C	-1.4193068425	-1.617215718	0.9299650424
C	-0.2145231433	-2.2982172287	1.0266602286
H	0.0317591813	-2.8124552321	1.9520008994
H	0.2107557197	-2.7583584788	0.1415732988
C	1.4229796048	-0.8485954243	0.8247699231
H	1.3849370543	-0.676685398	1.8989185859
C	2.5286607733	-1.7707941281	0.3548732945
C	0.9982793856	0.2048346914	0.0126808191
H	1.4754064599	0.3252922256	-0.9583248079
C	0.4258675461	1.4467894645	0.6491136676
C	-3.125095051	-0.1020678929	-0.2067336156
H	-2.0403991177	-1.54704598	1.8201124623
C	-3.251539894	0.9093530793	0.9538305202
C	-4.2310912382	-1.1755236126	-0.0571100521
C	-3.3809110015	0.6465192747	-1.5280280764
H	-4.3832796555	1.0872954818	-1.5153747912
H	-3.3211784751	-0.0271779047	-2.3885830175
H	-2.6697146627	1.4630234382	-1.6843072684
H	-4.1476060784	-1.7151380358	0.890460713
H	-4.1703978746	-1.9110329447	-0.8657083553
H	-5.222502449	-0.7092469519	-0.0912571312
H	-4.2580013789	1.3429890571	0.9729651466
H	-2.5373158957	1.7282798252	0.8390913969
H	-3.0736066696	0.440454415	1.9257571388

H	1.1786314209	1.8679056928	1.3341049436
H	-0.4175051339	1.152908852	1.2897218825
C	-0.0048200392	2.5382402804	-0.3316702122
H	0.8305311857	2.7680587404	-1.0085576185
C	-0.4644942021	3.8290980397	0.353866254
H	-0.8106677658	2.1557543695	-0.9674390335
H	0.362847767	4.2379538005	0.9495921204
H	-1.2642560376	3.5974191834	1.070237639
C	-0.9591342992	4.8848112153	-0.6386472748
H	-0.1727289463	5.153036092	-1.3535084535
H	-1.2750231946	5.8014606083	-0.1301163306
H	-1.8136015684	4.5108500847	-1.2145461007
C	3.9246817789	-1.1374888697	0.5022208852
H	2.3520067617	-2.0321908055	-0.6971065115
H	2.5089524445	-2.7150967409	0.9150025648
H	3.9662147492	-0.2226677285	-0.1042762724
C	5.0834847477	-2.0678306725	0.1121616075
H	4.0546575439	-0.817266899	1.5445434812
C	5.098710243	-2.4588052955	-1.3701844815
H	5.0417933561	-2.9754358954	0.7300913017
H	6.0310074115	-1.5734303109	0.3616445934
H	5.9784617843	-3.0642466482	-1.6113568781
H	5.1208739496	-1.5683488593	-2.0094713492
H	4.2143191662	-3.0417591538	-1.6466109853
H	4.2143191662	-3.0417591538	-1.6466109853

TS endo 0204

E(RB3LYP) = -706.412073248 A.U.

First frequency = -505.8122 cm^{-1}

H	-1.7121352632	-0.8384967907	-2.1948611877
C	-1.3681869645	-1.1562308377	-1.2151368691
H	-0.6125810602	-1.9301852221	-1.2482049384
C	-2.1893566188	-1.0140473147	-0.1005655249
C	-1.644753793	-1.3412318046	1.1618282482
C	-0.369270616	-1.8585155201	1.312974495
H	0.0401914052	-1.9871521158	2.3112187968
H	0.036536567	-2.5403755285	0.5748183992

C	1.0459927394	-0.384126772	0.381517396
H	1.018483918	0.1680855875	1.3162083993
C	2.2355578057	-1.3022335148	0.1938561975
C	0.422438752	0.1945537469	-0.7250645552
H	0.8187472504	-0.0682682681	-1.705672416
C	-0.2586203825	1.5396338179	-0.6389577131
C	-3.6178731008	-0.4423703858	-0.2429706011
H	-2.1585551475	-1.0051917958	2.0564482959
C	-4.4784742762	-1.5335488697	-0.9268452438
C	-3.6618730344	0.8347898245	-1.1085238726
C	-4.2608270011	-0.1059211399	1.1160241825
H	-3.6902872276	0.6579707646	1.6548254883
H	-4.3451672202	-0.9882823275	1.7579319927
H	-5.272173813	0.2833277852	0.9595993461
H	-3.2230544297	0.6820878449	-2.0983003724
H	-3.1298660572	1.6579941526	-0.6252337696
H	-4.7014539855	1.1468815635	-1.2582632791
H	-4.0921036832	-1.7694557885	-1.923176935
H	-5.517511822	-1.1995943739	-1.0328076578
H	-4.4737849744	-2.4574162078	-0.339273201
H	-0.8607603385	1.5750379729	0.2771739214
H	-0.9620665253	1.645082899	-1.4693951251
C	0.7033266134	2.7499290357	-0.6892711926
H	1.303867727	2.6787708145	-1.6062310542
C	1.6455054561	2.9298734461	0.5102321404
H	0.0940360846	3.658975343	-0.794417227
H	2.297156419	3.7899084532	0.3090243976
H	2.3076448289	2.0613497169	0.5911497692
C	0.9230486253	3.1537600374	1.8430662911
H	0.3226767754	2.2852976296	2.1332286543
H	0.2455279589	4.0137784967	1.7837920375
H	1.6353302051	3.3452637295	2.6523259346
C	3.5503706874	-0.5416023043	-0.0526131164
H	2.04683799	-1.9687666524	-0.6605972218
H	2.3640622042	-1.9536296921	1.0677485273
H	3.4286352264	0.1121397244	-0.9266199417
C	4.7546620699	-1.466047757	-0.2626730634
H	3.7474904531	0.1240504054	0.799380492

C	6.0586979842	-0.7004157054	-0.5043924841
H	4.5542439689	-2.1315661217	-1.1135487756
H	4.8670678524	-2.119227107	0.6134446932
H	6.2974979601	-0.0516133919	0.3460626768
H	5.9817558199	-0.0630546566	-1.3926817663
H	6.9039733632	-1.3801956282	-0.6533465795
H	6.9039733632	-1.3801956282	-0.6533465795

TS endo 0209

E(RB3LYP) = -706.411710229 A.U.

First frequency = -520.0747 cm⁻¹

H	-2.0398514068	-0.1622752864	-2.0644921727
C	-1.4616223602	-0.7543313834	-1.3643508816
H	-0.7183834694	-1.3821525616	-1.8424587591
C	-2.0006766612	-1.1294277128	-0.1354130365
C	-1.1510717621	-1.8078533024	0.7673114
C	0.1466957482	-2.173029244	0.4579311834
H	0.7796644301	-2.589353209	1.2358437201
H	0.4114796194	-2.4769610958	-0.5473559887
C	1.2134909744	-0.2439098555	-0.251303665
H	1.4552015313	-0.080515609	0.7944358191
C	2.3006125635	-0.8360414514	-1.127084395
C	0.2216040513	0.5626009048	-0.8107615344
H	0.3152164655	0.7972666269	-1.8695444901
C	-0.453435828	1.604170737	0.0526103566
C	-3.4170534045	-0.7199691307	0.3214042744
H	-1.4671049806	-1.8961093392	1.8042239592
C	-3.4038047325	0.0823772765	1.6428683797
C	-4.2219352047	-2.0243828133	0.5416713102
C	-4.1523784139	0.125707378	-0.7339274129
H	-3.6328129458	1.0695874447	-0.9297001577
H	-5.1585863517	0.3701066949	-0.3779770012
H	-4.257073815	-0.4104984938	-1.6823464018
H	-4.265189874	-2.6144580778	-0.3794938649
H	-5.2482690859	-1.7964090311	0.8524950374
H	-3.7646164699	-2.6481367996	1.3157322762
H	-2.9034999968	-0.45820073	2.4508525554

H	-4.43027341	0.2832430545	1.9699755104
H	-2.89831713	1.0432450914	1.516414696
H	-0.7618584166	1.1207251667	0.9866915868
H	-1.3693949844	1.9643806069	-0.4318869148
C	0.4480577977	2.8082820969	0.3893615714
H	-0.0898848321	3.4718971277	1.081078343
C	0.8938646836	3.6159379719	-0.8348190841
H	1.3363599898	2.4528985752	0.9289109864
H	0.0063388673	3.9411374196	-1.3955852004
H	1.4610143584	2.965008545	-1.5122100159
C	1.745537324	4.8335551674	-0.4652945329
H	1.1922490513	5.5190728007	0.1869685455
H	2.0551981172	5.3946482771	-1.3531497746
H	2.6522484042	4.5301141751	0.0707418162
C	3.3467151646	-1.6989407669	-0.4060752104
H	2.8279619095	-0.01639195	-1.6390551063
H	1.8345662179	-1.4232567583	-1.9328292737
H	2.8563145746	-2.5370681946	0.1036482637
C	4.2054054155	-0.9258632724	0.6035885636
H	4.0095759914	-2.1474476219	-1.1580962752
C	5.2695753948	-1.8040276422	1.2680728982
H	3.5658000686	-0.4846111147	1.3780771315
H	4.6878852016	-0.0816853136	0.0920315372
H	5.8735250077	-1.2350305554	1.9823147103
H	5.9491094154	-2.232690097	0.5224931513
H	4.8087199473	-2.6377075095	1.8103664755
H	4.8087199473	-2.6377075095	1.8103664755

TS endo 0211

E(RB3LYP) = -706.411550681 A.U.

First frequency = -520.1753 cm⁻¹

H	-1.5136449733	-0.1595070772	-2.1570754455
C	-1.0804648291	-0.705751017	-1.3269880812
H	-0.2086166507	-1.2880589385	-1.6024454583
C	-1.8675826754	-1.1013518628	-0.2477032273
C	-1.2125189383	-1.7133889802	0.8446498398
C	0.1413381912	-1.996536853	0.853705146

H	0.6001066925	-2.3625005061	1.7671741188
H	0.6501915627	-2.29414979	-0.055159952
C	1.2276200233	-0.0138565974	0.366931105
H	1.2205033805	0.1767602375	1.4374245913
C	2.5227432342	-0.5440044166	-0.2142724257
C	0.3469281915	0.7228784681	-0.4262323121
H	0.6685744791	0.9502359219	-1.4408394311
C	-0.5730070076	1.7269054008	0.2304518375
C	-3.3735852677	-0.7798806826	-0.1428405049
H	-1.7553657559	-1.8102694724	1.7820910871
C	-3.8934062512	0.0003080733	-1.3637112341
C	-3.7168350609	0.0400316016	1.1220661679
C	-4.1265631229	-2.1313774269	-0.0768756157
H	-5.2089886949	-1.9672400646	-0.0190551253
H	-3.8252050409	-2.7124778685	0.7999865125
H	-3.9179869768	-2.7361415724	-0.9653320579
H	-3.3851045068	-0.4545882003	2.0389359136
H	-4.8015746641	0.1765037719	1.1976787917
H	-3.2560453358	1.0306006046	1.087720767
H	-3.7403589001	-0.5545403758	-2.2946788056
H	-3.4020657492	0.9741567978	-1.4607727914
H	-4.9680312005	0.1816282075	-1.2579553221
H	-1.0566465706	1.2350650923	1.0822733743
H	-1.374046698	2.0169879629	-0.4606421524
C	0.1469393595	2.995085298	0.7295269746
H	-0.57703279	3.6272677443	1.2628655512
C	0.8050588289	3.8178030114	-0.3840212226
H	0.9103390017	2.7097352127	1.4658818024
H	0.0488924153	4.0717594056	-1.1400893213
H	1.5540068971	3.2011924087	-0.8970063936
C	1.4663905377	5.0978138157	0.134304393
H	1.9321211159	5.6686571877	-0.675777424
H	2.2451301472	4.8668935516	0.8703385608
H	0.7342096572	5.7498869359	0.6244202695
C	3.3960579415	-1.3286911345	0.7729810469
H	3.1137205342	0.3026751361	-0.5971395739
H	2.2986028194	-1.1599044926	-1.0975271716
H	3.5432128782	-0.7130586736	1.6706464359

C	4.7675024233	-1.7316969944	0.2108519938
H	2.8669059414	-2.2301447658	1.1045924473
C	4.6947126424	-2.721739559	-0.9576324424
H	5.3628682967	-2.1755371447	1.0187435521
H	5.3086719516	-0.8296214957	-0.1064096394
H	4.141712179	-3.6242841916	-0.6717434939
H	5.6948492124	-3.0309597949	-1.2781147515
H	4.1913555618	-2.2880818615	-1.8276901903
H	4.1913555618	-2.2880818615	-1.8276901903

TS endo 0224

E(RB3LYP) = -706.411754445 A.U.

First frequency = -522.1627 cm^{-1}

H	-1.4513693136	-0.8017415245	-2.1302405099
C	-0.986325433	-1.0596248449	-1.185554349
H	-0.1879131984	-1.7864957409	-1.2831292922
C	-1.7026856092	-0.9706736665	0.0065754325
C	-1.0002388732	-1.2208649083	1.2068104589
C	0.3251330062	-1.6143630595	1.2404414554
H	0.835521176	-1.6776651455	2.1966397356
H	0.7310413685	-2.2592932252	0.4705202643
C	1.5002629592	-0.0422115534	0.0071851265
H	1.5990553134	0.5107912292	0.9381487643
C	2.69805721	-0.8658402198	-0.419306161
C	0.6029973573	0.4483923111	-0.9426341345
H	0.8539598553	0.2865735136	-1.9905068299
C	-0.1842360065	1.69942996	-0.6347132918
C	-3.1649332266	-0.480949262	0.0755228055
H	-1.464033097	-0.9269321662	2.1457443289
C	-3.3264310101	0.7756298194	0.9622441076
C	-4.0058231743	-1.6294821694	0.6850430519
C	-3.739738777	-0.1514931614	-1.3139473228
H	-3.1926537858	0.6659170866	-1.7953290276
H	-4.7843757712	0.1623981996	-1.2183562562
H	-3.7129834306	-1.0198281197	-1.9797506656
H	-3.6689972293	-1.8771714014	1.6961836276
H	-3.9252018826	-2.5353866431	0.0755939311

H	-5.0632404562	-1.3454381168	0.7404875582
H	-2.9331706252	0.6241541158	1.9710806685
H	-4.3871093853	1.0338414927	1.0585127091
H	-2.8115980882	1.6348649448	0.5249851272
H	-0.5861487424	1.6022130713	0.3794413154
H	-1.047470908	1.785943118	-1.3062358895
C	0.6599659843	2.9827348288	-0.7383173323
H	1.5002867294	2.9172779497	-0.0339938361
C	-0.1346072348	4.2707998226	-0.4723371967
H	1.1062937634	3.0343073589	-1.7404426421
H	-0.9675837211	4.3348558288	-1.1861795276
H	0.5109621401	5.1337393819	-0.6800705698
C	-0.6775051177	4.3852691257	0.9570494849
H	-1.4065210892	3.6000506569	1.1810866547
H	-1.1736885126	5.3481893471	1.1163040281
H	0.1328225964	4.301682417	1.6908955923
C	3.6007849244	-1.3274423869	0.7318622272
H	3.3084994066	-0.2725088756	-1.1178461473
H	2.3534939795	-1.7316050052	-1.0037923722
H	3.8725172508	-0.4489435848	1.3325780381
C	4.8832071314	-2.0386071291	0.2748605233
H	3.0417975175	-1.9931191047	1.4005207173
C	4.6345184886	-3.3705347945	-0.4427270527
H	5.5179916883	-2.2183670527	1.1517296196
H	5.454451315	-1.3690386172	-0.3828774502
H	5.5769839925	-3.8712952216	-0.6869067791
H	4.085008549	-3.2319091401	-1.379339286
H	4.0484079106	-4.0504905418	0.186777624
H	4.0484079106	-4.0504905418	0.186777624

TS endo 0246

E(RB3LYP) = -706.413014618 A.U.

First frequency = -525.7408 cm⁻¹

H	-1.3204657725	0.2297939801	-2.031017493
C	-1.1352078457	-0.5866915857	-1.3432759651
H	-0.4357940292	-1.3213376164	-1.7196968115
C	-2.0691060814	-0.9345875535	-0.3738513476

C	-1.7068751794	-1.932457184	0.5589139155
C	-0.5081328917	-2.6288813319	0.4796028806
H	-0.2439573584	-3.3215854132	1.2745167541
H	-0.1203794866	-2.9098308267	-0.4935856456
C	1.1448050553	-1.1969702977	0.5230129207
H	1.1411784781	-1.2421143559	1.6110976222
C	2.2344448699	-2.0132695574	-0.1430134554
C	0.7005520653	0.000534249	-0.044910794
H	1.1450383869	0.3108214574	-0.9856203078
C	0.1397779149	1.0715937273	0.8572493472
C	-3.4180617014	-0.2006281317	-0.200465245
H	-2.3009071112	-2.035739688	1.4641498217
C	-4.5386360391	-1.2690753162	-0.2294347773
C	-3.6963516272	0.7960138112	-1.3409767837
C	-3.495545576	0.5659915096	1.1389505065
H	-2.7806044366	1.3928858654	1.1621755231
H	-3.2885824361	-0.0840638695	1.9938731705
H	-4.4979862241	0.987281274	1.2768894356
H	-2.9734152335	1.6170257513	-1.355903452
H	-4.688992227	1.2397154644	-1.2105655493
H	-3.6744805648	0.3035433175	-2.3182238226
H	-4.5126714349	-1.8337756257	-1.1669509361
H	-5.5221903213	-0.7930592493	-0.1429198937
H	-4.4394456543	-1.9838446278	0.5923928692
H	0.8746289468	1.2917913499	1.645002339
H	-0.7236163805	0.6479393864	1.3869640214
C	-0.2590078007	2.3798513629	0.164018761
H	-1.0262389388	2.1630557286	-0.5867052834
C	0.897021867	3.1370795596	-0.5126659799
H	-0.7276936883	3.0427058669	0.9040535586
H	0.483078053	4.0153794411	-1.0240836399
H	1.3386378879	2.5141439844	-1.3010599713
C	1.9993630415	3.590675435	0.4506479061
H	2.5106794121	2.7398511457	0.9122906142
H	1.5869570014	4.2063223084	1.2586716423
H	2.7580321597	4.1850809002	-0.0687457063
C	3.6619588924	-1.5493231373	0.2165588411
H	2.1053817381	-1.9681827223	-1.2341728225

H	2.1413875498	-3.0706449483	0.1343232713
H	3.7875970736	-1.5953204852	1.3077471109
C	4.0305882179	-0.1444287511	-0.2727594887
H	4.3774773454	-2.2710383449	-0.2016394579
C	5.4743405396	0.2399546638	0.0626451782
H	3.345111435	0.5877808793	0.1682028631
H	3.8753094485	-0.0881298069	-1.3593514487
H	5.7131929289	1.2483787953	-0.2906910707
H	6.1876934457	-0.453502111	-0.3974244541
H	5.6453513518	0.2172722184	1.1451576674
H	5.6453513518	0.2172722184	1.1451576674

TS endo 0256

E(RB3LYP) = -706.412425830 A.U.

First frequency = -503.5530 cm^{-1}

H	-1.184918526	-0.7316597545	-2.1068269548
C	-1.0122099439	-1.1851011435	-1.1352833076
H	-0.358591878	-2.0467888303	-1.1665442601
C	-1.947467828	-1.0392552102	-0.1150720891
C	-1.6135935237	-1.5510899205	1.1593557479
C	-0.4413661145	-2.2493261202	1.3982914325
H	-0.1819161151	-2.5257258919	2.4165946612
H	-0.0349599144	-2.9097196889	0.641213082
C	1.2680628173	-0.9171291592	0.8033552409
H	1.2062953981	-0.4601523502	1.7893248681
C	2.3475488144	-1.967515748	0.6472651743
C	0.8374023541	-0.1408789946	-0.2736235393
H	1.3000397966	-0.3161984344	-1.2419382858
C	0.2853756566	1.2420347856	-0.0283641928
C	-3.2625971949	-0.265640724	-0.3607746407
H	-2.1931368616	-1.233342748	2.0198148902
C	-4.040232345	0.0111634679	0.9398139163
C	-4.1474623564	-1.1516955097	-1.2723875466
C	-3.0326935857	1.0895897188	-1.0641502738
H	-2.4888357843	1.7827504704	-0.4175736497
H	-3.9965010121	1.5476028022	-1.3126214924
H	-2.4719730001	0.9850600421	-1.996956132

H	-5.1144715085	-0.6707201245	-1.4617145692
H	-4.3341314609	-2.1245123547	-0.8059417833
H	-3.6608217238	-1.3313119291	-2.235950208
H	-4.3149565642	-0.9140142191	1.4558957387
H	-4.9672992539	0.5460076762	0.7089544277
H	-3.4620304017	0.6323957779	1.6319863537
H	-0.4737861609	1.1759867922	0.7640540154
H	-0.2289906839	1.5975780759	-0.9242138135
C	1.3525524246	2.2702726039	0.3925210715
H	1.9126467424	1.872414277	1.2478660343
C	0.7731776436	3.6449486826	0.7613639564
H	2.0814804037	2.3896807504	-0.4216102944
H	1.584937114	4.2806765177	1.1375387542
H	0.068660076	3.5237365361	1.5959537489
C	0.070970135	4.3630241876	-0.3971832004
H	-0.2553031116	5.3655457654	-0.1017551328
H	-0.8148096423	3.8171312609	-0.7376219588
H	0.7433924423	4.4705600291	-1.2565391879
C	3.7808023712	-1.4135221381	0.8129972703
H	2.2463004707	-2.4513498699	-0.3332592033
H	2.2129104043	-2.7621964449	1.3911660725
H	3.8543845879	-0.9393448316	1.8009608521
C	4.242079631	-0.4122782443	-0.2563877701
H	4.4786158913	-2.2625644166	0.8284334501
C	4.3279944906	-1.0014584564	-1.6683653217
H	5.2299910802	-0.0306266488	0.0314450528
H	3.5698288416	0.4527372598	-0.2600162447
H	4.7230375016	-0.268406694	-2.3792588322
H	3.3477142393	-1.3193663212	-2.0381343215
H	4.9867137864	-1.8776360117	-1.6909518951
H	4.9867137864	-1.8776360117	-1.6909518951

TS endo 0259

E(RB3LYP) = -706.412209049 A.U.

First frequency = -499.5470 cm^{-1}

H	-1.7509279221	-0.1823988439	-2.2178305892
C	-1.3397713272	-0.8387127023	-1.4566883775

H	-0.7025856267	-1.6192265078	-1.8514893815
C	-1.994495874	-1.0025494509	-0.2404170507
C	-1.3534067386	-1.7795742287	0.7521640793
C	-0.155620174	-2.4372701122	0.5295943611
H	0.3472241682	-2.9274113114	1.3587923546
H	0.0617010413	-2.868404783	-0.4404612459
C	1.3413723212	-0.8757838979	-0.1128918983
H	1.5175361306	-0.681597998	0.9419058676
C	2.3406311831	-1.7804029928	-0.8021649901
C	0.6582319075	0.1042691164	-0.8303674043
H	0.8758078598	0.191863196	-1.8936019227
C	0.1753122575	1.3544071061	-0.1381669725
C	-3.3352357949	-0.2837235449	0.0320943628
H	-1.7057735927	-1.7133374583	1.7762408915
C	-4.413302935	-0.9921894522	-0.8251812927
C	-3.2988704823	1.209983978	-0.3578621535
C	-3.7650011602	-0.368432164	1.5090209643
H	-3.0359578679	0.1118264486	2.1702265805
H	-3.8967397298	-1.4040817536	1.8373780818
H	-4.7235706365	0.1430276518	1.6444800719
H	-2.6136690507	1.7694859072	0.2838460595
H	-4.2971650256	1.6474359858	-0.2461035317
H	-2.9914955124	1.3621370283	-1.3960262512
H	-5.4004916175	-0.5464175091	-0.6547341558
H	-4.4704144	-2.0567596215	-0.5757132811
H	-4.1813350574	-0.9111349919	-1.8915683765
H	-0.3690368959	1.0617016835	0.7707841819
H	-0.5417815687	1.874947144	-0.7774821567
C	1.311871467	2.3181008183	0.2515601269
H	2.037897227	1.7772424695	0.8709138927
C	0.8325870806	3.5654443286	1.0105810825
H	1.8533610521	2.6258431301	-0.6541930954
H	1.7100832598	4.1380789387	1.3372567952
H	0.315723221	3.2498333518	1.9275641053
C	-0.0885022164	4.4827791977	0.197420966
H	-0.3369911932	5.390426041	0.7571013146
H	-1.0308020095	3.9889162844	-0.0607365963
H	0.3916929827	4.7893098994	-0.7393866199

C	3.6971808232	-1.0989037633	-1.0824945959
H	1.9193085729	-2.1156180502	-1.7601698878
H	2.5061096315	-2.687894083	-0.2101335701
H	4.3475773495	-1.8160549486	-1.6029227399
C	4.4273085857	-0.5733132047	0.1634653558
H	3.5323687178	-0.2638375404	-1.7751165179
C	4.7323069167	-1.6499154874	1.2105240616
H	3.8312872243	0.2242271491	0.6235337949
H	5.3659434644	-0.1034165611	-0.1562965573
H	5.3237503189	-1.2423362147	2.036771665
H	5.2989450356	-2.4793717356	0.7711894224
H	3.8154384383	-2.0681823511	1.6392130993
H	3.8154384383	-2.0681823511	1.6392130993

TS endo 0266

E(RB3LYP) = -706.411183270 A.U.

First frequency = -521.5456 cm⁻¹

H	-1.6200221093	0.0349780549	-2.1653426166
C	-1.2068466215	-0.6157648424	-1.4031830619
H	-0.3773506167	-1.2184754781	-1.7552279106
C	-2.0000896509	-1.0727596273	-0.3525526449
C	-1.3662493611	-1.8289958911	0.6588414386
C	-0.0316736848	-2.1894561276	0.6119613478
H	0.4163713836	-2.6718992937	1.4753390053
H	0.4462752958	-2.4221772245	-0.3318258408
C	1.1647779788	-0.2308830868	0.291596184
H	1.1901656204	-0.1510818153	1.375602923
C	2.4146765971	-0.7722456198	-0.3732138803
C	0.3119836605	0.6298741672	-0.40079839
H	0.6283160681	0.9427864466	-1.3941312053
C	-0.533632762	1.6131821479	0.3762900741
C	-3.4821926375	-0.6761974044	-0.1835908512
H	-1.9001703846	-1.9894605701	1.5926652524
C	-4.3144994508	-1.9807813821	-0.2404860245
C	-3.9723753935	0.2552491571	-1.3068428625
C	-3.7562029794	0.027222558	1.1655853809
H	-4.8292883857	0.2197666106	1.2770010029

H	-3.2356102867	0.9865781155	1.2236413485
H	-3.4427332528	-0.5788039084	2.0198655711
H	-5.0323150293	0.4873496644	-1.1600514214
H	-3.8676347691	-0.2082957285	-2.2928180018
H	-3.4246061694	1.2034450664	-1.3142675811
H	-4.1566687557	-2.5012345251	-1.1906664979
H	-5.3840042035	-1.7604378032	-0.1427240982
H	-4.0352727319	-2.6664075294	0.5653172614
H	-1.0252665472	1.0677312096	1.1899861981
H	-1.3320165483	2.0139674733	-0.2604029795
C	0.2703353343	2.7840597245	0.9749268392
H	-0.4030566997	3.400263814	1.5873532668
C	0.9496348577	3.6742747165	-0.0720406507
H	1.0324676471	2.3854245099	1.6580543813
H	0.1924209103	4.0432082088	-0.7780562124
H	1.6494467488	3.0704317234	-0.6635788051
C	1.6962669778	4.8582084032	0.5486639666
H	2.4774081796	4.5130057821	1.2358043043
H	1.0149448216	5.4984735423	1.1208261748
H	2.1751946537	5.4793247667	-0.2154390854
C	3.2788285575	-1.6646137053	0.5259966415
H	3.017888261	0.0771872012	-0.722383129
H	2.1423396933	-1.3257230719	-1.2863533202
H	3.5628180786	-1.0949198238	1.4225230061
C	4.5465376299	-2.2055003154	-0.1527722701
H	2.6790630656	-2.5101332594	0.8804494188
C	5.5676900287	-1.1275607947	-0.5349864693
H	4.2602347459	-2.7734794554	-1.0488192955
H	5.0254146136	-2.9259453082	0.5223961065
H	5.1707348755	-0.4363214318	-1.2851547337
H	6.4770284275	-1.5741608924	-0.9501603513
H	5.8567787491	-0.5346524186	0.3407158612
H	5.8567787491	-0.5346524186	0.3407158612

TS endo 0277

E(RB3LYP) = -706.411183422 A.U.

First frequency = -524.3755 cm^{-1}

H	-1.5937265127	-0.7096665318	-2.2392545754
C	-1.1247750356	-0.9951915582	-1.3044065866
H	-0.267801425	-1.646576836	-1.4342840904
C	-1.8678246807	-1.0551186357	-0.126288819
C	-1.1685482574	-1.3346816358	1.0683699211
C	0.186427534	-1.6085546355	1.1058452577
H	0.6821998022	-1.697988612	2.0676162011
H	0.66469649	-2.1542510928	0.3014522642
C	1.2212197608	0.1553394672	0.0265611907
H	1.2299657901	0.649295641	0.9934286871
C	2.5129962006	-0.5143862328	-0.398710988
C	0.3208897252	0.6209465289	-0.9353778611
H	0.6310994751	0.5261172869	-1.9765151262
C	-0.5739753163	1.8038983989	-0.6408476132
C	-3.365565158	-0.6901100894	-0.0542000611
H	-1.6733628221	-1.1540080025	2.0147282813
C	-3.9461551632	-0.3149671309	-1.429591528
C	-3.6342027049	0.4870251566	0.9115980359
C	-4.1217619517	-1.9389022443	0.4616655474
H	-3.9653568539	-2.7915922702	-0.2069799804
H	-5.1984066451	-1.740450963	0.5194591087
H	-3.7782750524	-2.230144593	1.4587990332
H	-3.2625950468	0.2861334308	1.9200616591
H	-4.7116960005	0.6716389148	0.9895744874
H	-3.1606500354	1.4053889305	0.5555253145
H	-5.0151512587	-0.0980404093	-1.3341743027
H	-3.8352310092	-1.1300873949	-2.1516700462
H	-3.4653710891	0.576980723	-1.8446611443
H	-0.9232683265	1.7330240748	0.3950891747
H	-1.4708821358	1.7612960289	-1.2684592168
C	0.1051115217	3.1711589717	-0.8810277538
H	0.4402314139	3.2126215876	-1.9263261472
C	1.2908577624	3.5086986871	0.0357225148
H	-0.6573406172	3.9557526247	-0.7743748229
H	1.732395992	4.4543223074	-0.3040271604
H	2.0716605815	2.7477898575	-0.0803603726
C	0.9158796466	3.6384867293	1.5159408624
H	0.1339795181	4.3937507017	1.6582317481

H	1.7802268696	3.9349989649	2.1191500852
H	0.5378350996	2.6963604415	1.9256513543
C	3.421591608	-0.9448685192	0.7596768834
H	3.0800703739	0.179415323	-1.0388297617
H	2.282158974	-1.3751504455	-1.0433743727
H	3.5730893388	-0.080195301	1.4199535802
C	4.7899758704	-1.4823035171	0.3150203556
H	2.9179672815	-1.7073083043	1.365922579
C	4.7154070997	-2.7854964034	-0.4892532397
H	5.4101194074	-1.6467838748	1.205256993
H	5.3057582703	-0.7145917664	-0.2781506122
H	4.1870174087	-3.5633922286	0.0744970115
H	5.7154308115	-3.1645617304	-0.7235260422
H	4.1864377237	-2.6485846226	-1.4378806989
H	4.1864377237	-2.6485846226	-1.4378806989

TS endo 0279

E(RB3LYP) = -706.411056145 A.U.

First frequency = -524.6996 cm^{-1}

H	-1.4128804419	-0.336489503	-2.2154704663
C	-1.034019341	-0.8336520647	-1.3296707892
H	-0.2933635035	-1.5948664144	-1.5477189753
C	-1.8207625913	-0.938275752	-0.1834753311
C	-1.2232624154	-1.5055136756	0.964083816
C	0.0620582651	-2.0165591245	0.9747140463
H	0.4983982328	-2.3315739745	1.9177631915
H	0.4672370781	-2.5153255359	0.1027223967
C	1.4395321171	-0.3328093763	0.1660778779
H	1.5282633048	-0.0108061099	1.2007544373
C	2.5885285469	-1.1516496352	-0.3866158684
C	0.6415321693	0.4347844622	-0.6836894124
H	0.9423175426	0.4900108172	-1.729442356
C	-0.0679038187	1.6496434113	-0.1347923722
C	-3.2407311014	-0.3414802854	-0.0803548716
H	-1.7253207021	-1.3810536037	1.9208435681
C	-3.684177938	0.3485780638	-1.3830062477
C	-3.3687765539	0.6885680446	1.0658040935

C	-4.2116925813	-1.5152240196	0.1982195784
H	-4.1595024666	-2.260727321	-0.6018432269
H	-5.2446454952	-1.1539110695	0.264662807
H	-3.9681892892	-2.0184583591	1.1388595741
H	-2.7476594285	1.5682979931	0.8789424727
H	-3.0771451219	0.2702401003	2.0329203814
H	-4.4083935737	1.0238106362	1.1540308003
H	-3.6783535911	-0.3434426958	-2.230964357
H	-3.040189554	1.1988644329	-1.6312333054
H	-4.704702397	0.7294636742	-1.2719809786
H	-0.5201226313	1.3781113611	0.8274720423
H	-0.8916077053	1.9334418852	-0.7973417612
C	0.8660080681	2.8550989667	0.0746908452
H	1.7140693313	2.5403922578	0.6956776069
C	0.1787085161	4.0635495406	0.7297954291
H	1.2914847802	3.1567910897	-0.8931057253
H	0.933417306	4.8365139031	0.9235805285
H	-0.2108387073	3.7641548703	1.7126734221
C	-0.9565617916	4.6705190799	-0.1031764437
H	-1.3572207839	5.5721185766	0.3715294037
H	-1.7885270909	3.9701053988	-0.229303027
H	-0.6038811886	4.9484250926	-1.1034800163
C	3.4036028364	-1.9001521132	0.6750644325
H	3.2559080758	-0.4821877358	-0.9467059084
H	2.2107198813	-1.869976839	-1.1321303787
H	3.8005704811	-1.1711245473	1.3960885986
C	4.5622764808	-2.7351132698	0.1088307879
H	2.7379590133	-2.5586445142	1.2439392298
C	5.6679191925	-1.9099269771	-0.5600411903
H	4.1625003464	-3.4634088271	-0.6103734766
H	5.0012765871	-3.3240225254	0.9241221746
H	6.0725834367	-1.1633510294	0.1333876167
H	5.3018589768	-1.3762100596	-1.442813876
H	6.4966083241	-2.5481725626	-0.88354475
H	6.4966083241	-2.5481725626	-0.88354475

TS endo 0285

E(RB3LYP) = -706.411735960 A.U.

First frequency = $-525.6374 \text{ cm}^{-1}$

H	-1.0097828749	-0.0059935697	-1.9750365114
C	-0.7925611105	-0.6405499749	-1.1237675725
H	0.087185708	-1.2559157856	-1.2542738872
C	-1.8020161506	-1.0442560701	-0.2549896095
C	-1.4206199543	-1.7653824742	0.8987662334
C	-0.10591982	-2.1031526363	1.1732831793
H	0.1420562068	-2.5484482863	2.1329981403
H	0.5693983158	-2.3742394709	0.3706748037
C	1.074535796	-0.1880533485	1.1715433002
H	0.7234123734	-0.0092813062	2.1855645466
C	2.4802392673	-0.7618044019	1.0999641996
C	0.5274656978	0.6326213966	0.1816637543
H	1.1245676456	0.8349111027	-0.7029085901
C	-0.4467160978	1.716374441	0.5845976674
C	-3.276811408	-0.6208958316	-0.4267345195
H	-2.1519563547	-1.8906976399	1.693749797
C	-3.4916231618	0.2665197123	-1.6660136611
C	-3.8178158178	0.1456933284	0.8018070054
C	-4.1068293327	-1.9150975969	-0.6095098601
H	-4.0232161227	-2.5688719298	0.263967193
H	-3.7607139589	-2.4785897854	-1.4820336601
H	-5.1670519351	-1.6759804342	-0.7532372206
H	-3.2989466507	1.0991077701	0.9315549724
H	-3.7093204485	-0.4258691877	1.727465969
H	-4.8847832855	0.3593696607	0.6714366032
H	-3.18423081	-0.2405319196	-2.5859911958
H	-2.9359013365	1.2071140466	-1.5911183627
H	-4.5530843723	0.5170179912	-1.7633440129
H	-1.1758300744	1.2843197076	1.2791298569
H	-1.0163024967	2.0615475238	-0.2850491734
C	0.2317099444	2.9208509985	1.2714186125
H	-0.5406504577	3.6610661328	1.5240882345
C	1.3294735676	3.6017343296	0.4387785817
H	0.6660809512	2.5854578544	2.2219026075
H	2.1521129152	2.8930132484	0.2784338489
H	1.7508796274	4.4294519873	1.0231660101

C	0.8451979984	4.1334962346	-0.9144809486
H	0.0012078748	4.8219128607	-0.7886368827
H	0.5123950946	3.3225695001	-1.5710697404
H	1.6414499087	4.6734745635	-1.4371142132
C	3.0157467896	-1.0791702472	-0.301884571
H	2.5397569898	-1.6704808362	1.7139047695
H	3.1665629224	-0.0447871392	1.5773611083
H	2.3289724099	-1.7594530182	-0.8235940414
C	4.4136530776	-1.7075903157	-0.2743152312
H	3.0497728818	-0.1628655953	-0.9052296096
C	4.9594663433	-2.0096703294	-1.6726279988
H	4.3826071387	-2.6324422423	0.3174589567
H	5.1017794856	-1.0328070528	0.252871894
H	5.9568699658	-2.4587074251	-1.627228138
H	5.0316390361	-1.0958147713	-2.2734158236
H	4.3042339538	-2.7054342244	-2.2092397449
H	4.3042339538	-2.7054342244	-2.2092397449

TS endo 0289

E(RB3LYP) = -706.411046828 A.U.

First frequency = -525.0498 cm^{-1}

H	-1.3226915159	-0.3212622153	-2.0822336452
C	-1.0294095942	-0.8711848903	-1.1956980024
H	-0.1739597948	-1.5153263269	-1.346724249
C	-1.9505865221	-1.1616268292	-0.1942206115
C	-1.4638190052	-1.7705272592	0.9844412616
C	-0.1316285611	-2.1047663212	1.1625099227
H	0.2049680048	-2.457234679	2.1337690553
H	0.458557431	-2.4688656468	0.3299433048
C	1.0577866023	-0.2255278804	0.8598382007
H	0.7969229052	0.0689168462	1.8742371953
C	2.4483563047	-0.827350195	0.7349074763
C	0.4391644166	0.498298727	-0.1632386601
H	0.9561155174	0.5841286947	-1.1142914332
C	-0.476094077	1.645848761	0.2029079486
C	-3.4303797342	-0.7263305921	-0.2621206813
H	-2.1136756059	-1.8002829651	1.8558352618

C	-3.7579193769	0.0370741591	-1.5579836649
C	-3.8370739885	0.1707029979	0.9293511947
C	-4.2889650695	-2.0143426918	-0.2296197371
H	-5.3554671103	-1.7682577744	-0.2921098118
H	-4.1258648981	-2.5788501014	0.6934674016
H	-4.0380667513	-2.6697036387	-1.06994974
H	-3.6426105543	-0.3072942572	1.8931779597
H	-4.9093063836	0.3927771823	0.883759579
H	-3.2975077517	1.121332524	0.909561256
H	-3.5505120831	-0.5661655563	-2.4473760682
H	-3.1859458835	0.9677388092	-1.634133942
H	-4.8207058586	0.2999818075	-1.5751286831
H	-1.1577423866	1.3023870453	0.9891751579
H	-1.1007386731	1.9261325051	-0.6542112898
C	0.2765369741	2.8933915682	0.707508283
H	-0.4575589847	3.6479299287	1.0239226267
C	1.2186602799	3.5147782926	-0.3298772685
H	0.8531196783	2.6271163285	1.6039106689
H	0.6491226152	3.7486779325	-1.2403052693
H	1.9732727062	2.7742945074	-0.6241667069
C	1.9160486546	4.7783792421	0.1813694311
H	2.5144568869	4.5624521274	1.074025237
H	1.1862317019	5.5494777005	0.4539181943
H	2.5852790263	5.2042217109	-0.5735108341
C	2.8611764501	-1.2841466416	-0.6714215806
H	2.5485743204	-1.6772664578	1.4238185677
H	3.1683758596	-0.0770373374	1.0922804689
H	2.0908205127	-1.9495162893	-1.0814830692
C	4.2136076264	-2.012604479	-0.7129936512
H	2.9036926635	-0.4177382704	-1.3443881675
C	5.4074369239	-1.1403365394	-0.3077199785
H	4.376819257	-2.3918684527	-1.7296857949
H	4.1674009868	-2.8960946939	-0.0616339936
H	6.3508252862	-1.6836356769	-0.4235163017
H	5.3404605359	-0.8180354587	0.7361400004
H	5.4627038354	-0.2389939415	-0.9295065266
H	5.4627038354	-0.2389939415	-0.9295065266

TS endo 0292

E(RB3LYP) = -706.411072335 A.U.

First frequency = -526.4920 cm^{-1}

H	-1.2147607317	-0.0652455803	-2.1289263515
C	-0.8900977892	-0.6794301085	-1.297198147
H	0.0120321577	-1.2411935633	-1.4977036453
C	-1.7977090101	-1.1366043085	-0.3464620815
C	-1.2792528516	-1.8249965524	0.7731343583
C	0.0722988235	-2.079217908	0.9386121416
H	0.4246730755	-2.5027150936	1.8753369037
H	0.6941511465	-2.3167103052	0.0837973256
C	1.1278010734	-0.1014492166	0.8407416123
H	0.8464077371	0.0649672416	1.8784431338
C	2.5553289727	-0.5945878793	0.6647515352
C	0.4592189854	0.6805817491	-0.1052613505
H	0.9699164169	0.9085374626	-1.0359922812
C	-0.5440897691	1.7069346776	0.3727486151
C	-3.3049076504	-0.8054168232	-0.3968565247
H	-1.9333761141	-1.9893984488	1.6261251696
C	-4.0652304814	-2.1489035653	-0.5158426228
C	-3.673587827	0.0648760712	-1.6118195554
C	-3.791469989	-0.0716149389	0.8737383424
H	-3.3233290637	0.9120973533	0.9648938677
H	-3.5745952633	-0.6339625141	1.7858623152
H	-4.8765067738	0.0761035074	0.8299090302
H	-4.7526018516	0.2508444473	-1.6212000973
H	-3.4127477502	-0.4246648412	-2.5553463093
H	-3.1709028808	1.0372213586	-1.5799281002
H	-3.756096421	-2.6919772508	-1.4147819287
H	-5.1463396915	-1.976234501	-0.5732152418
H	-3.8711449344	-2.7939941807	0.3464623187
H	-1.1983973858	1.2276387958	1.1096509691
H	-1.1869211028	2.0285557431	-0.4559069835
C	0.1052314347	2.9476201863	1.0176707804
H	-0.6876066848	3.6009832758	1.4086621075
C	0.993159959	3.7537105296	0.0627500127
H	0.7018444824	2.6317914665	1.8843514243

H	0.4059142434	4.0394029957	-0.8212714631
H	1.8055053011	3.1138207795	-0.3047132441
C	1.5852380968	5.0058913594	0.7153251495
H	2.1996507577	4.74260617	1.5840670678
H	0.7949484889	5.6805107117	1.0643817843
H	2.2170984743	5.5650446884	0.0173565923
C	2.9986305006	-0.8816876113	-0.7766784594
H	2.7045055106	-1.4908561038	1.2782260349
H	3.2348536259	0.1627872714	1.0867868954
H	2.3082298706	-1.5944807247	-1.248004817
C	4.4298332828	-1.4319189574	-0.8858883759
H	2.9307312285	0.0409105732	-1.365438081
C	4.6070640167	-2.8399959491	-0.3057500847
H	5.1216157428	-0.7385616759	-0.3880564751
H	4.7210609744	-1.4445680514	-1.9437033101
H	5.6258876214	-3.207550892	-0.4654186207
H	3.9183936752	-3.5478499149	-0.7818172914
H	4.4146338594	-2.8665079691	0.7713618468
H	4.4146338594	-2.8665079691	0.7713618468

TS endo 0300

E(RB3LYP) = -706.411052794 A.U.

First frequency = -527.6908 cm^{-1}

H	-1.0870500263	-0.5180244268	-2.1868073738
C	-0.8326122502	-0.9570602716	-1.2291690422
H	-0.0584461699	-1.7098080994	-1.2885927986
C	-1.7553240389	-0.9882877608	-0.1876775618
C	-1.3091329715	-1.4632726053	1.0659444822
C	-0.0184669086	-1.9171262664	1.2811119003
H	0.3029788231	-2.1537796415	2.2918250857
H	0.504406997	-2.4687900479	0.5090369639
C	1.3662247317	-0.2537717448	0.6765577566
H	1.1734425629	0.2101102866	1.6415991791
C	2.6755687603	-1.0236044505	0.6161929513
C	0.7940266346	0.3814803365	-0.4292397776
H	1.2935924854	0.2897110226	-1.3904298575
C	0.0135264278	1.6572605451	-0.2139884174

C	-3.1781978295	-0.4006152198	-0.3072356565
H	-1.9349196912	-1.2851345029	1.9373991873
C	-4.1762271561	-1.5541324313	-0.041880395
C	-3.4625501729	0.1662120254	-1.7098012684
C	-3.438261619	0.7267888798	0.718235342
H	-2.8036487233	1.5938251713	0.5172880846
H	-3.2520533354	0.4033625518	1.7458552654
H	-4.4821960071	1.0552422412	0.660479874
H	-4.49016821	0.5413959162	-1.7570506022
H	-3.3509932958	-0.5977832634	-2.4855828224
H	-2.7956086474	1.0002472581	-1.9520540462
H	-4.0292111486	-2.3675102318	-0.7597886155
H	-5.209181076	-1.1982496925	-0.132413119
H	-4.0491151138	-1.9692836939	0.9624548084
H	-0.6383674299	1.5142781451	0.6541567847
H	-0.6436856211	1.8601326642	-1.068723351
C	0.9234359406	2.8780794336	0.0170854004
H	1.5500098935	2.6956457798	0.9008455772
C	0.159913625	4.1999633555	0.1922337324
H	1.6143869506	2.9701800835	-0.8316405673
H	-0.4609403601	4.3785731664	-0.6966565085
H	0.8836524732	5.0242948522	0.228317312
C	-0.7189091668	4.2516849273	1.4475688893
H	-1.1866862983	5.2348062192	1.563541252
H	-0.1256460187	4.055672113	2.3485401001
H	-1.5220916331	3.5086884816	1.4147768004
C	2.9767365036	-1.7410813425	-0.7074397691
H	2.7085706742	-1.7609370512	1.4300071361
H	3.4888722498	-0.3156759731	0.8320190357
H	2.1235622416	-2.3734075376	-0.9836394539
C	4.2409273205	-2.6138512712	-0.6643428543
H	3.0815749322	-1.0034428356	-1.5136895987
C	5.5382416763	-1.8278078693	-0.4420142667
H	4.3166294206	-3.1684828236	-1.6081816381
H	4.1304227217	-3.3695809571	0.1253622702
H	6.4118516664	-2.4858598764	-0.4907754195
H	5.5532979477	-1.3344682857	0.5349229909
H	5.6616643451	-1.0518039477	-1.2066156055

H 5.6616643451 -1.0518039477 -1.2066156055

TS endo 0303

E(RB3LYP) = -706.412422815 A.U.

First frequency = -522.7650 cm⁻¹

H	-0.9785689052	-0.0537053328	-2.1372195129
C	-0.874086602	-0.7753419682	-1.3363166141
H	-0.2428507096	-1.6170032029	-1.589353991
C	-1.8451723414	-0.8983221587	-0.3487501686
C	-1.5878800045	-1.7896328222	0.7173278684
C	-0.4436689889	-2.5710867445	0.7774365335
H	-0.2509488446	-3.1635651559	1.6680620896
H	-0.034695442	-2.9975638969	-0.1316464172
C	1.2999676219	-1.2318302072	0.6991571156
H	1.2202960152	-1.0711823163	1.7732896738
C	2.3619480131	-2.2303375238	0.2828618695
C	0.9864346673	-0.1380862787	-0.1130770978
H	1.4941060863	-0.0570795048	-1.0714296121
C	0.5143833518	1.1546948075	0.5107874464
C	-3.1301620255	-0.0413774956	-0.3174146106
H	-2.2122139117	-1.7310742105	1.6052228175
C	-4.3247313036	-1.0115111187	-0.4907473386
C	-3.1817349324	0.9908921945	-1.4580151218
C	-3.3036030292	0.7194878438	1.0166844401
H	-3.3151440769	0.0487122556	1.8797341234
H	-4.2529227146	1.2667598532	1.0153094443
H	-2.5002941261	1.445959337	1.1670157204
H	-4.1250218667	1.545063675	-1.413014412
H	-3.1262173113	0.5130189512	-2.4409545109
H	-2.368085706	1.7182547504	-1.3827477349
H	-4.3591284636	-1.7473751677	0.3184197402
H	-4.2462605634	-1.5584525119	-1.4358870065
H	-5.2725271138	-0.4604520706	-0.4901457903
H	1.2080121161	1.4322265147	1.3168728652
H	-0.4497192108	0.9760578805	1.0050991596
C	0.4059505006	2.3170780316	-0.4818944914
H	1.4119791389	2.5599345851	-0.8533650739

C	-0.2436666152	3.5851906396	0.0894291547
H	-0.1654155918	1.9852890761	-1.3558724164
H	-1.2710889579	3.3536634956	0.4017197348
H	-0.3320775521	4.3283234628	-0.7134038848
C	0.5179066564	4.2058356719	1.2661116613
H	0.0523805522	5.1425156313	1.5896081883
H	1.5553793799	4.4266357445	0.988574563
H	0.5431037067	3.5352995533	2.1309574486
C	3.7901538173	-1.8104666553	0.6975294131
H	2.3158393512	-2.3786165557	-0.8041619994
H	2.1622200874	-3.2114780592	0.7308603908
H	3.8097193997	-1.6929613805	1.7893823419
C	4.3281064024	-0.5260671277	0.0489035057
H	4.4749127648	-2.6386495956	0.4669030015
C	4.5105380135	-0.6232118968	-1.4694803155
H	5.2947091007	-0.2847725763	0.5091430986
H	3.6591940231	0.3100671819	0.2855248859
H	4.9469247932	0.295255156	-1.8753459799
H	3.559085872	-0.7885590342	-1.9851019818
H	5.1750471443	-1.4542994973	-1.7335338992
H	5.1750471443	-1.4542994973	-1.7335338992

TS endo 0309

E(RB3LYP) = -706.411736445 A.U.

First frequency = -512.9445 cm^{-1}

H	-1.9764137567	-0.2417365065	-2.0963446941
C	-1.4450005589	-0.8385879109	-1.364187985
H	-0.7227647864	-1.517680563	-1.8019243632
C	-2.0206866645	-1.1349397996	-0.1319482306
C	-1.2239629082	-1.8249036949	0.8107587573
C	0.0571181353	-2.2688336311	0.5390445787
H	0.6550833187	-2.6918114261	1.3406803937
H	0.3230631109	-2.6167274148	-0.4516757136
C	1.2357389082	-0.4218135261	-0.1872665521
H	1.4387557327	-0.2182215792	0.8593843306
C	2.3390768011	-1.09236684	-0.9813248025
C	0.3156517703	0.4099918007	-0.8246881436

H	0.4543503325	0.5769769913	-1.8912648975
C	-0.3235425128	1.5347599473	-0.04245161
C	-3.4190644386	-0.6317307037	0.2849426029
H	-1.5613534179	-1.8576480033	1.8441162361
C	-3.3818132315	0.2166031348	1.5768664051
C	-4.2986560179	-1.88083689	0.5374257685
C	-4.0891581856	0.2143885275	-0.8126609559
H	-3.5141527589	1.1201055491	-1.0323656342
H	-5.085522864	0.5270782304	-0.4834725911
H	-4.2089052992	-0.3493597453	-1.7431505889
H	-3.888908131	-2.5000971388	1.3411812052
H	-4.3604015541	-2.5009222001	-0.3627231958
H	-5.3154034572	-1.5854518081	0.8218378012
H	-4.4005514225	0.4847376996	1.8789359779
H	-2.822821189	1.1435938253	1.4245904035
H	-2.9240813586	-0.320044509	2.41220249
H	-0.7126862334	1.1182180925	0.8935969568
H	-1.1846624637	1.9384339739	-0.5893341019
C	0.6496198445	2.6824981553	0.2930747977
H	0.1270577316	3.4220196578	0.9161680921
C	1.2354872993	3.3857561778	-0.9363771258
H	1.4715702286	2.2876506873	0.9058335522
H	0.4148533989	3.759139146	-1.5648551173
H	1.7791362637	2.6541733622	-1.5475705893
C	2.1725149082	4.5397914711	-0.569594582
H	2.5810759871	5.0276347099	-1.4606948661
H	3.0165673745	4.182932861	0.0320107454
H	1.6490296161	5.3023918591	0.0185392068
C	3.2709886132	-2.0289946661	-0.1934144794
H	2.9512244497	-0.3097190644	-1.4517935783
H	1.8974695822	-1.6486899065	-1.821457784
H	2.7253665866	-2.9292950629	0.1108209038
C	3.9231532303	-1.400338391	1.0502590111
H	4.0634449574	-2.3680643856	-0.8739289439
C	4.6757136159	-0.0949957808	0.7697249056
H	4.614130608	-2.1332434048	1.4854935622
H	3.1596587507	-1.2207639329	1.8176911254
H	5.4249530473	-0.2320784396	-0.0188389311

H	5.1948469269	0.2624278208	1.664812422
H	3.9943219432	0.6984633344	0.4450441316
H	3.9943219432	0.6984633344	0.4450441316

TS endo 0311

E(RB3LYP) = -706.411118782 A.U.

First frequency = -529.5474 cm⁻¹

H	-1.0297754606	-0.4418392318	-2.2129830926
C	-0.7252263122	-0.8706755451	-1.2653738881
H	0.0949023186	-1.5705879314	-1.3494749168
C	-1.621191462	-0.9718721625	-0.2047446464
C	-1.1171835671	-1.4265448691	1.0342138336
C	0.2042301367	-1.7992810027	1.2166046106
H	0.5631095386	-2.0213991337	2.2180037252
H	0.7429418707	-2.3122365992	0.4290925711
C	1.4690139108	-0.0481372039	0.589062883
H	1.2789837585	0.3892407415	1.5668941279
C	2.8172162653	-0.7417743308	0.4790069947
C	0.8227183306	0.5646005193	-0.4880992747
H	1.2977042014	0.5236265149	-1.4650888894
C	-0.0361458707	1.7796000261	-0.2252624801
C	-3.0821653816	-0.4790759127	-0.2884630353
H	-1.7333274056	-1.2958741573	1.9208211318
C	-3.995109489	-1.6988122691	-0.01280147
C	-3.4342567193	0.0786079016	-1.6793050402
C	-3.3947969839	0.620281906	0.7527359353
H	-4.4598796084	0.8765286844	0.7216700522
H	-2.8261404703	1.5303911529	0.5450676907
H	-3.1629720257	0.3029763326	1.772993587
H	-2.8295544802	0.9570460197	-1.9279592645
H	-4.4852895068	0.3849615915	-1.7009845714
H	-3.2893669612	-0.6700918414	-2.4644310103
H	-5.0512230057	-1.4121711361	-0.0784115499
H	-3.8189203485	-2.1122507951	0.9848084997
H	-3.8096314559	-2.4949809374	-0.7410272188
H	-0.6522306227	1.574618193	0.6565330543
H	-0.7294655677	1.9529813575	-1.0576919541

C	0.7931714094	3.0561360158	0.0077709295
H	1.4579318709	2.8996840857	0.8682898004
C	-0.0555748529	4.3164393442	0.236547999
H	1.449395998	3.2150995588	-0.8584314147
H	-0.715922096	4.4687269407	-0.628453709
H	0.6090176225	5.1892924327	0.2691963922
C	-0.8946837117	4.2796002243	1.5193133328
H	-0.2600797073	4.107772036	2.3967444087
H	-1.6442423543	3.4822605755	1.4945289344
H	-1.4264530949	5.224408747	1.6721342044
C	3.1154546507	-1.4360245351	-0.8574809043
H	2.9147054899	-1.4663979231	1.2959480373
H	3.6052237837	0.0068616749	0.6587037178
H	2.3266415095	-2.1652487899	-1.0870365059
C	4.4758170743	-2.1510653892	-0.8928749607
H	3.0874065907	-0.6943572535	-1.6645464597
C	4.5689597769	-3.3701790596	0.0322278533
H	5.2671584609	-1.4331880658	-0.6367929775
H	4.6772608611	-2.4708849343	-1.9229813997
H	3.7803476922	-4.0961901155	-0.1980098497
H	4.4651335205	-3.0935333177	1.0860752409
H	5.5324232147	-3.8779762662	-0.0795102335
H	5.5324232147	-3.8779762662	-0.0795102335

TS endo 0322

E(RB3LYP) = -706.411201701 A.U.

First frequency = -540.0395 cm⁻¹

H	-1.6021023723	-0.9631227164	-2.193595686
C	-1.2813643005	-1.2789974984	-1.2073993984
H	-0.7436836962	-2.2197712555	-1.2111236621
C	-1.9912996807	-0.8928551094	-0.070896759
C	-1.454001901	-1.2543499287	1.1839252667
C	-0.3012563359	-2.0102538544	1.3143632719
H	0.1391112602	-2.1508459657	2.2978105489
H	-0.0930189826	-2.8115417812	0.6157379583
C	1.3073494069	-0.9557087552	0.1179948754
H	1.5166954488	-0.3555104992	0.9951148137

C	2.2223813986	-2.1441026103	-0.0991177262
C	0.7102273461	-0.3315009974	-0.9826036362
H	0.9479337605	-0.7591358986	-1.9560460045
C	0.430444952	1.1641210913	-1.0265887548
C	-3.2561119741	-0.0097674953	-0.1297450362
H	-1.8472514335	-0.7675524841	2.0735823124
C	-4.4198328069	-0.8392374526	0.4666573899
C	-3.6344334344	0.3805418157	-1.5699263668
C	-3.1067935566	1.2933962684	0.6861626112
H	-2.8293595841	1.1028940626	1.7263997018
H	-4.0542600711	1.844002801	0.6947652241
H	-2.3464992405	1.9433494013	0.2481704328
H	-2.8508543412	0.978332135	-2.047688102
H	-4.5491638196	0.9823230364	-1.5626959171
H	-3.820477993	-0.4995402529	-2.1933722254
H	-5.3559244964	-0.2695500729	0.4326826767
H	-4.2239876748	-1.1065559457	1.5094299208
H	-4.5626277669	-1.7683233375	-0.0945223574
H	-0.5333067738	1.3543079709	-1.5143118273
H	1.1855845269	1.6258280437	-1.6819550494
C	0.4545666988	1.8918999965	0.3219921397
H	-0.2421850156	1.4046769902	1.0138923537
C	0.1107027154	3.3801257625	0.1989317436
H	1.4505924375	1.799202798	0.7745923327
H	-0.8588484618	3.4942006532	-0.3046202871
H	0.846265301	3.8673619054	-0.4556948533
C	0.0683690215	4.0927074381	1.5532171597
H	-0.6923470877	3.6472568959	2.2044981975
H	-0.1666846203	5.1563507294	1.4433631545
H	1.0315809143	4.0146526152	2.0703401779
C	3.6057719533	-1.7571092313	-0.6600816935
H	1.7463879686	-2.8455296454	-0.7992874034
H	2.3619714771	-2.6928876835	0.8411031919
H	4.1812338066	-2.6735732642	-0.8526260258
C	4.4176149126	-0.8400425952	0.2619553959
H	3.4725087032	-1.263920891	-1.6325206687
C	5.8044443253	-0.5127517335	-0.298459678
H	4.5191712871	-1.3166097378	1.2470362937

H	3.8617080785	0.0910982675	0.4289627045
H	6.3658238651	0.14513381	0.3730697075
H	5.7268207543	-0.0103689906	-1.2695748227
H	6.3964081107	-1.423418395	-0.4458877348
H	6.3964081107	-1.423418395	-0.4458877348

TS endo 0325

E(RB3LYP) = -706.412396377 A.U.

First frequency = -524.4746 cm⁻¹

H	-1.5669968851	-0.3659456542	-2.0980850272
C	-1.2561284783	-0.9488663235	-1.2394253689
H	-0.6382594724	-1.8002388352	-1.4933523854
C	-1.9950912706	-0.9421743934	-0.0621788816
C	-1.4705822966	-1.6417735474	1.0485726758
C	-0.312774349	-2.4018437076	0.9765092011
H	0.0930333467	-2.8390207136	1.8850722214
H	-0.1046581916	-2.976101784	0.0807369727
C	1.3226245343	-1.099406351	0.2806610336
H	1.5060478769	-0.820753832	1.315311212
C	2.2491995162	-2.1521052801	-0.2959986197
C	0.7936017099	-0.1054018393	-0.5445916592
H	1.0638934462	-0.1210588781	-1.5990696436
C	0.441037742	1.2385813852	0.0455499514
C	-3.2892547798	-0.1178914233	0.1181539569
H	-1.8882402623	-1.4379983271	2.0319705445
C	-3.1236529742	0.9933627602	1.1781522733
C	-4.4018911607	-1.0897866108	0.5821872751
C	-3.7597185567	0.5368419131	-1.1936744223
H	-4.710579327	1.0543111312	-1.0286351976
H	-3.9154706625	-0.2075964298	-1.9807741179
H	-3.0456580618	1.2793936971	-1.562066568
H	-5.3517089904	-0.5552436061	0.6989616531
H	-4.1590955209	-1.5552749716	1.5416629252
H	-4.5473985612	-1.8911183104	-0.1493988199
H	-2.7833065873	0.5963716756	2.1386736871
H	-4.0795190729	1.5018349597	1.3486741117
H	-2.400570706	1.7434139034	0.848406383

H	1.3382242186	1.6420211764	0.5365612593
H	-0.2898024691	1.0869675912	0.852130472
C	-0.0833633214	2.261816005	-0.9651394981
H	0.6485184971	2.3676817432	-1.7790702607
C	-0.3779141044	3.6494498047	-0.3750203064
H	-0.9933044896	1.8648099254	-1.4266140818
H	-1.0916333652	3.5498381847	0.453873943
H	-0.8836852231	4.2550870202	-1.1377339075
C	0.865255818	4.401779805	0.1143355108
H	0.6070299198	5.4058150653	0.4665391724
H	1.6000241538	4.5093906274	-0.6921925985
H	1.3575670732	3.8809063523	0.9416816198
C	3.6590194184	-1.6216661661	-0.6240987036
H	1.8042373852	-2.5551723418	-1.216755262
H	2.340360931	-2.9977649884	0.3979115292
H	4.2386400596	-2.4240859134	-1.1018599811
C	4.4310856782	-1.1050671036	0.5954937624
H	3.5745391135	-0.8156517076	-1.365426448
C	5.8460935973	-0.6359419389	0.2458129263
H	4.4809861696	-1.8987442083	1.3540322618
H	3.8751902029	-0.2781778383	1.0547286673
H	6.4373865389	-1.4515067823	-0.186264649
H	6.3790903447	-0.2688145304	1.1289860908
H	5.8197884738	0.1764439747	-0.489560516
H	5.8197884738	0.1764439747	-0.489560516

TS endo 0327

E(RB3LYP) = -706.411670819 A.U.

First frequency = -522.8169 cm^{-1}

H	-1.3381654343	-0.1350263032	-2.1029710252
C	-1.0283844942	-0.7372749591	-1.2577042098
H	-0.3144496608	-1.5096451929	-1.5123800252
C	-1.8381792018	-0.8713964905	-0.1358714004
C	-1.3212020243	-1.5898804103	0.966310378
C	-0.0799709352	-2.2076818413	0.9415703493
H	0.3059451138	-2.6605597179	1.8511667755
H	0.265703873	-2.6846992871	0.031437199

C	1.4327923818	-0.6757163862	0.4702668195
H	1.4879311409	-0.4174491186	1.5260936361
C	2.5413420617	-1.5772279899	-0.0339376485
C	0.8652029002	0.2786371204	-0.3760856046
H	1.2284838665	0.3228628331	-1.4016860955
C	0.2950531376	1.5553657463	0.1952928997
C	-3.2215316081	-0.1957776413	-0.0073054283
H	-1.8300264692	-1.5074694199	1.9234025217
C	-3.5747613895	0.669040256	-1.230592072
C	-3.3305210279	0.6962935792	1.2500351278
C	-4.2710205498	-1.3295142799	0.0998757171
H	-4.2353475028	-1.9758140674	-0.7830899943
H	-5.2819671696	-0.9129833902	0.1803678474
H	-4.0910181806	-1.9559019384	0.9788802889
H	-2.6310749938	1.5353482114	1.2033108731
H	-3.1292672127	0.1429452201	2.1710726215
H	-4.3425382854	1.1086987615	1.3308893633
H	-3.5739619941	0.0836498271	-2.1552265571
H	-2.8780539115	1.5037849434	-1.3513052469
H	-4.5774005369	1.0915997608	-1.1077472414
H	1.0441688113	2.0104586848	0.8583363437
H	-0.5531218761	1.301127694	0.8451055809
C	-0.1256972979	2.576924049	-0.8666322191
H	0.7687311086	2.9071204689	-1.4142972917
C	-0.8632566195	3.8052625162	-0.3150462505
H	-0.7635316866	2.0782953841	-1.6047417835
H	-1.7895414814	3.4787344226	0.1768083211
H	-1.1750357721	4.4362663328	-1.1572352998
C	-0.0372186649	4.6473019533	0.6638743351
H	0.2115269603	4.0864363494	1.5703815939
H	-0.5823956751	5.5454505427	0.9719003118
H	0.9052053589	4.9692384895	0.205277973
C	3.9023571807	-0.8591220732	-0.0954132868
H	2.2870721608	-1.939744305	-1.0410895426
H	2.6246205023	-2.4660459725	0.6016401363
H	3.7945865252	0.0345547435	-0.7226925145
C	5.0496623324	-1.7263729308	-0.6366188912
H	4.1620493442	-0.4965702844	0.9093525249

C	5.4134769014	-2.9180963159	0.2566851423
H	5.9368867461	-1.0934069579	-0.7658270432
H	4.7852154366	-2.0877875756	-1.6400923646
H	4.5879918826	-3.6320880988	0.3406586212
H	5.6666256582	-2.5845836788	1.2699304797
H	6.276944823	-3.4614881385	-0.140709689
H	6.276944823	-3.4614881385	-0.140709689

TS endo 0335

E(RB3LYP) = -706.411629465 A.U.

First frequency = -524.5820 cm^{-1}

H	-1.3567051339	0.4210937305	-1.9688479411
C	-1.1237312337	-0.4098575509	-1.3140450435
H	-0.3441651433	-1.057557656	-1.6934388336
C	-2.0573643302	-0.88977759	-0.4034420679
C	-1.6414605697	-1.9011392515	0.492089401
C	-0.3783888975	-2.4756619413	0.4372464104
H	-0.0839665287	-3.1809226292	1.2102001509
H	0.0806375024	-2.6648712406	-0.5268367614
C	1.1210666307	-0.8839932347	0.6175609447
H	1.0895205578	-0.9929266849	1.7000236789
C	2.3004227001	-1.5446371401	-0.0649309391
C	0.5825935107	0.2937600522	0.0953484807
H	1.0233747106	0.7009953241	-0.8098602977
C	-0.1377443467	1.2481493115	1.0174211571
C	-3.4739238849	-0.2908699751	-0.2563245645
H	-2.262736834	-2.1136868591	1.3588787564
C	-4.4845959134	-1.4321099523	-0.527737626
C	-3.7450101344	0.8357639818	-1.2697732147
C	-3.7315920455	0.2731131972	1.1593102491
H	-3.0912787097	1.1357308935	1.3637276065
H	-3.5536032322	-0.4715615865	1.939842831
H	-4.7729527808	0.6025502929	1.2492881096
H	-4.7722525245	1.1973465721	-1.1549898998
H	-3.6281649267	0.488025405	-2.3009707803
H	-3.0768797385	1.6884772404	-1.1164005061
H	-5.5130951992	-1.0586294039	-0.4608709238

H	-4.3733716701	-2.2463298595	0.1945436694
H	-4.3364728268	-1.8516049999	-1.5280719157
H	0.5096362329	1.4748391946	1.8786385251
H	-0.9928262854	0.7066541189	1.4418444089
C	-0.5940453342	2.5725577959	0.3810679579
H	-0.8920313804	2.3892495708	-0.6585287424
C	0.4568706491	3.6954505426	0.4206830852
H	-1.4937326189	2.9319123896	0.896061284
H	0.6830829113	3.9312303288	1.4696694529
H	0.0147811894	4.6049649158	-0.0063380376
C	1.7643774415	3.3803279262	-0.3143760743
H	1.576960413	3.1315462954	-1.3656186195
H	2.2855720015	2.5310175078	0.1386720978
H	2.4452937386	4.2376006227	-0.2913876872
C	3.6286544794	-0.8180203083	0.2086085151
H	2.1263205897	-1.5698985381	-1.1507356159
H	2.3936319055	-2.5904648097	0.2553346263
H	3.5461923401	0.2208714503	-0.1384027521
C	4.83552125	-1.4880495606	-0.4572514724
H	3.7932642962	-0.7625234088	1.2938846178
C	6.1509197146	-0.7525220943	-0.1854055558
H	4.663082163	-1.547069002	-1.5407101929
H	4.9133648536	-2.5258809752	-0.1055234949
H	6.361873912	-0.7076312205	0.8891865066
H	6.1090119175	0.278206365	-0.5556525468
H	6.9979220715	-1.2476880763	-0.6713877451
H	6.9979220715	-1.2476880763	-0.6713877451

TS endo 0336

E(RB3LYP) = -706.410397457 A.U.

First frequency = -525.8175 cm^{-1}

H	-1.8788156352	-0.7367402481	-2.1315599335
C	-1.3824472362	-1.1733431635	-1.2722656104
H	-0.7334782041	-2.0036602315	-1.5288541252
C	-1.9762670233	-1.1225148879	-0.0106226969
C	-1.2294010704	-1.6215970538	1.0796153686
C	0.011057631	-2.2170095864	0.9386692669

H	0.5812982449	-2.4743474256	1.826405135
H	0.2405642557	-2.8191091697	0.0687532663
C	1.3173312202	-0.708864175	-0.2570207133
H	1.5753805742	-0.3063838849	0.7164768949
C	2.3055320077	-1.6696327056	-0.890735184
C	0.4305758149	0.0261298131	-1.0461899127
H	0.5646966505	-0.0347454913	-2.1259185967
C	-0.1022099908	1.3392058855	-0.5229600609
C	-3.3286842928	-0.4273224992	0.2551446527
H	-1.5619311063	-1.3771417055	2.0859797161
C	-3.214101045	0.7108950198	1.2955106408
C	-4.2976921481	-1.5037452763	0.803229862
C	-3.9458288405	0.1659925308	-1.0242245798
H	-4.9138444073	0.6218890486	-0.791864519
H	-4.1144992027	-0.6011723077	-1.7864880112
H	-3.3097965452	0.9450189816	-1.4575067116
H	-3.9281189511	-1.9324250898	1.7396859112
H	-4.4154005769	-2.3221192703	0.0855691479
H	-5.2862518959	-1.0705648705	0.9957808492
H	-4.2066441126	1.1215991358	1.512850658
H	-2.5882719511	1.5258132878	0.9229737043
H	-2.7892806424	0.3651670403	2.2417774379
H	-0.4301910016	1.1896647793	0.5130062525
H	-0.9898744132	1.6456679304	-1.089663369
C	0.9361631624	2.4731022993	-0.5608810668
H	1.8140969532	2.178515858	0.029577335
C	0.3876586531	3.80356935	-0.0332326934
H	1.2949702507	2.6077142414	-1.5911522402
H	0.0239820127	3.6603695626	0.9936155717
H	-0.4895485873	4.0944555122	-0.627339583
C	1.4240053023	4.9305379466	-0.059664019
H	2.2966765435	4.6765634635	0.5529030624
H	1.0096771202	5.8692831559	0.3224226904
H	1.7804497493	5.113475058	-1.0798754024
C	3.3401632818	-2.2805331318	0.07448298
H	2.8425440149	-1.1573178904	-1.7031592478
H	1.7488125241	-2.4770767997	-1.390159472
H	2.8628350361	-2.4761460233	1.0431440278

C	4.6019269935	-1.4263958246	0.2875226299
H	3.6561463465	-3.2574892846	-0.3109777649
C	4.3571822899	-0.0369513452	0.8865184224
H	5.1180489	-1.3150382254	-0.6761026037
H	5.2911179358	-1.9807683495	0.9377309518
H	3.8297651225	-0.1059508258	1.8451589018
H	3.7533119919	0.5874258834	0.2209950376
H	5.3030984795	0.4854653744	1.0639081349
H	5.3030984795	0.4854653744	1.0639081349

TS endo 0345

E(RB3LYP) = -706.410847670 A.U.

First frequency = -506.5657 cm⁻¹

H	-1.8595649339	-0.3520718972	-2.1023573531
C	-1.3209200281	-0.807793346	-1.2766219489
H	-0.4605799348	-1.387367031	-1.5875494931
C	-1.9811645283	-1.1014925129	-0.0870171201
C	-1.2063387476	-1.5934712905	0.9885265328
C	0.1398248278	-1.8916713841	0.8743287576
H	0.6981144071	-2.1645367358	1.7645385963
H	0.5404589141	-2.2922229152	-0.0491763182
C	1.184569418	0.0119447387	0.1023062456
H	1.3044004655	0.2785863008	1.1493445881
C	2.3972944849	-0.5905168614	-0.5793441809
C	0.2332059687	0.7107213271	-0.6366375022
H	0.4282858702	0.8458825514	-1.6983310673
C	-0.6097917631	1.7674944403	0.0384616233
C	-3.4913813815	-0.8134060049	0.0644490831
H	-1.6315582575	-1.5796018231	1.9868148265
C	-3.8777696297	0.5986239918	-0.425565057
C	-3.9795692867	-0.9521900639	1.5189440789
C	-4.2420938456	-1.8589131186	-0.7974264124
H	-5.327202446	-1.7271791425	-0.7106598113
H	-3.9939225858	-2.8764138323	-0.4781722609
H	-3.9700428232	-1.7644831676	-1.8532036907
H	-3.8146849282	-1.9608121384	1.9104747349
H	-5.0550782832	-0.7529422404	1.5679448421

H	-3.4793325304	-0.2395222067	2.1831841159
H	-3.5565451786	0.7847137736	-1.453944056
H	-3.4393739917	1.3710362772	0.2109615889
H	-4.9667020705	0.7169391294	-0.397486185
H	-1.0954931488	1.3144272758	0.9129318444
H	-1.4111671253	2.0895449496	-0.6346375063
C	0.1899033201	3.0046507248	0.4934869056
H	-0.4854505931	3.6859962172	1.0300406402
C	0.8614628643	3.7645886396	-0.6558830756
H	0.9564093008	2.6966012127	1.2171384017
H	0.0989977824	4.0485360749	-1.3947591126
H	1.5548749502	3.0919583581	-1.1767257041
C	1.6141613345	5.0121733318	-0.185700911
H	2.4008545535	4.749265424	0.5309361264
H	0.938314633	5.7169068576	0.3124194301
H	2.0871319288	5.5378736517	-1.0217582179
C	3.3758513224	-1.3076972918	0.3566634533
H	2.9431251384	0.2099080899	-1.1017143248
H	2.0728635914	-1.2809224103	-1.3737857888
H	3.6715844181	-0.6185148727	1.160565096
C	4.6307677322	-1.8174547913	-0.3600186971
H	2.8760238514	-2.1505758596	0.8487189948
C	5.606950876	-2.5306742617	0.5797342173
H	5.1380084146	-0.9737851238	-0.8476360842
H	4.3324555913	-2.499769679	-1.1678414099
H	5.943929136	-1.8609808966	1.3792783771
H	6.494307642	-2.8854663301	0.0455848623
H	5.133972734	-3.3979736418	1.0545019252
H	5.133972734	-3.3979736418	1.0545019252

TS endo 0347

E(RB3LYP) = -706.411652137 A.U.

First frequency = -524.3813 cm^{-1}

H	-1.5716241985	0.2155074106	-1.967085493
C	-1.2746841318	-0.5798627717	-1.2942299713
H	-0.5910802989	-1.2920252109	-1.7384583828
C	-2.0786208023	-0.9503086328	-0.2225547999

C	-1.5720642684	-1.9190150332	0.6737468803
C	-0.3578955848	-2.5619494464	0.474934396
H	0.0231265302	-3.224487902	1.2477647126
H	-0.0556140609	-2.838094665	-0.5289149496
C	1.2157852287	-1.0250216358	0.2957770675
H	1.3414508701	-1.0659360511	1.3746840403
C	2.2398104177	-1.7889509984	-0.5206791339
C	0.64002655	0.1372354447	-0.2194552023
H	0.9490718393	0.4678718948	-1.2067582078
C	0.1083806938	1.1818829524	0.7329506569
C	-3.431530473	-0.2717978503	0.0876584992
H	-2.0625501118	-2.0399210814	1.6367431879
C	-3.4540570776	0.3914660761	1.4834922877
C	-4.5171592745	-1.3751019232	0.045153608
C	-3.802806053	0.8025118652	-0.9505280468
H	-3.8565769335	0.3861210726	-1.9612980797
H	-3.0831726804	1.6267399095	-0.9557875081
H	-4.7849464889	1.2238770715	-0.711841121
H	-4.3328460952	-2.1473571248	0.7979565215
H	-4.5363586508	-1.8628633741	-0.9347852919
H	-5.5082915349	-0.9468891188	0.2351058899
H	-4.4567458672	0.7769382812	1.7003313003
H	-2.7569177859	1.2326307298	1.5330336047
H	-3.1925653281	-0.3106410457	2.2798054821
H	0.883676384	1.4187189153	1.4778255618
H	-0.7026957875	0.7176064457	1.3077310507
C	-0.3648327376	2.4920171089	0.079773211
H	-0.8105312082	2.267466663	-0.8972988797
C	0.739382118	3.549620545	-0.0919325478
H	-1.1666940315	2.9328531052	0.6851364856
H	1.1099500581	3.8371484199	0.9016155692
H	0.2949936556	4.4555015931	-0.5241627733
C	1.9246015416	3.1087221988	-0.9583635209
H	2.4508812017	2.2567628912	-0.5160929772
H	2.6492044259	3.9211386619	-1.0765136556
H	1.5932970933	2.8093446979	-1.959701941
C	3.5842681749	-1.0487958009	-0.6686785458
H	1.8345352221	-1.9757911433	-1.5253204623

H	2.4184272727	-2.7746974101	-0.07236155
H	4.2510961554	-1.6436868821	-1.3084852666
C	4.2896765646	-0.7590358754	0.6608981487
H	3.412833251	-0.1010688705	-1.1968949748
C	5.6322971924	-0.0469313638	0.4745196464
H	4.4411222231	-1.7022863962	1.2040619983
H	3.6353373822	-0.1445710617	1.2917969611
H	6.3194192233	-0.6495127014	-0.1306261543
H	6.1199242165	0.1526122529	1.4343251665
H	5.4983051094	0.9129697033	-0.0376004367
H	5.4983051094	0.9129697033	-0.0376004367

TS endo 0351

E(RB3LYP) = -706.412050019 A.U.

First frequency = -520.9193 cm^{-1}

H	-1.5264421634	-0.0715145258	-2.1735905072
C	-1.1742699609	-0.75427688	-1.4100776125
H	-0.5567359458	-1.5555933902	-1.7946444129
C	-1.8643497334	-0.9117103186	-0.2137049961
C	-1.2890344294	-1.7445688577	0.7732434895
C	-0.1128275839	-2.448870708	0.5668779905
H	0.3335227436	-2.9921260749	1.395767379
H	0.0928340941	-2.8818996937	-0.4053946199
C	1.455024147	-0.9936797877	0.0227456613
H	1.6325972007	-0.8167542058	1.0808748487
C	2.4260588391	-1.9372534312	-0.6586355673
C	0.8782492333	0.05632204	-0.6936487301
H	1.130969353	0.1463622863	-1.7490231433
C	0.4836566719	1.3293746037	0.0174005814
C	-3.1658435142	-0.1482618461	0.1177306693
H	-1.6813016623	-1.6942547234	1.7858849552
C	-3.5883276787	0.8178630828	-1.003529955
C	-3.056924751	0.6651167407	1.4273436775
C	-4.2830532182	-1.2074461441	0.2858382603
H	-4.4012625836	-1.7952627794	-0.6301845275
H	-5.2413575721	-0.7245796657	0.5104116567
H	-4.0540472755	-1.9016686312	1.1000541014

H	-2.3039883456	1.4534142294	1.3430673788
H	-2.7931602927	0.0396994953	2.2843001064
H	-4.0169484132	1.1425062943	1.6537346209
H	-3.7382154261	0.2958218473	-1.9536214011
H	-2.8476906559	1.6080079024	-1.1582883878
H	-4.534620566	1.300813363	-0.738545536
H	1.3405984036	1.682275194	0.6083963697
H	-0.2988911839	1.0939806281	0.7510968366
C	0.0242078161	2.4498643545	-0.9213116144
H	0.8689279426	2.7448986567	-1.5603740694
C	-0.529582384	3.6926591369	-0.209932798
H	-0.7410767667	2.0539578344	-1.5978695984
H	-1.4105651058	3.4076055779	0.3809970081
H	-0.8904331422	4.4001109558	-0.9675100797
C	0.4831058069	4.4017650353	0.6963665261
H	0.7953364094	3.7654100936	1.5304462457
H	0.0605727289	5.3178077172	1.1219118634
H	1.3840693588	4.6782226176	0.1360561494
C	3.8121540041	-1.3080029289	-0.9149313891
H	2.0064732601	-2.2523155793	-1.6241576122
H	2.5447456159	-2.8520581774	-0.0665183725
H	4.456700226	-2.0609003381	-1.3900861519
C	4.5144015265	-0.7623424487	0.3384071707
H	3.6973360244	-0.4913966785	-1.6389157506
C	4.7467610954	-1.8120614863	1.4303798387
H	3.9263477901	0.0679152281	0.7494282406
H	5.4784083663	-0.3324604237	0.0385007884
H	3.8018124124	-2.1905767994	1.834399739
H	5.3170610741	-1.3947676684	2.2665682009
H	5.3056112851	-2.670770955	1.0400578858
H	5.3056112851	-2.670770955	1.0400578858

TS endo 0352

E(RB3LYP) = -706.412162494 A.U.

First frequency = -539.1632 cm^{-1}

H	-1.2408095476	0.1173254777	-2.0911533272
C	-0.831570629	-0.4724288883	-1.2792266089

H	-0.0577211281	-1.1618432571	-1.5929820483
C	-1.5817549378	-0.7317035985	-0.1366533396
C	-0.9437184591	-1.4101994076	0.9261610733
C	0.3390009406	-1.9268813413	0.8296219284
H	0.800438028	-2.3556567144	1.714314796
H	0.6724791738	-2.3662414442	-0.1037208832
C	1.7251206269	-0.2700129201	0.2295567163
H	1.9016421226	-0.0956505766	1.2887234558
C	2.8052383092	-1.042996376	-0.5046563309
C	0.9658591964	0.683452917	-0.4495401397
H	1.2127589858	0.8803299922	-1.4913683397
C	0.3430779317	1.8191064331	0.3243943042
C	-3.0244670993	-0.2170540976	0.0640789045
H	-1.4113392896	-1.3866446346	1.9080683415
C	-3.1223046143	0.7980598663	1.2242188611
C	-3.9136864131	-1.4408440151	0.3962971325
C	-3.5981394465	0.4428015532	-1.2036040054
H	-3.0520155037	1.3493022714	-1.480996757
H	-4.6402623197	0.7314796864	-1.0309203984
H	-3.5769197541	-0.2422837657	-2.0569541006
H	-3.8689985188	-2.1830111907	-0.4072589978
H	-4.9580523595	-1.1317806152	0.5202827991
H	-3.5973998057	-1.9320574536	1.3208764373
H	-2.7261645595	0.3908570691	2.158740898
H	-4.1681341566	1.075054606	1.3998023709
H	-2.5692648279	1.7114579646	0.9938852439
H	1.1368816686	2.343921327	0.878477264
H	-0.3187194466	1.3967667457	1.0938044403
C	-0.4131897973	2.8388073225	-0.5285031182
H	0.2421323293	3.1929810985	-1.3370932799
C	-0.9218790659	4.045106571	0.2676463614
H	-1.25702921	2.3431184611	-1.0209471974
H	-0.0666504011	4.572743517	0.7111664277
H	-1.5297366942	3.6957764708	1.1130965848
C	-1.7438900242	5.0153228073	-0.5851179066
H	-2.0894969228	5.8743469838	-0.0009437816
H	-2.627094712	4.5178103841	-1.0023031526
H	-1.1541227087	5.3981875738	-1.4259394529

C	3.6061774117	-2.0205448387	0.3625003188
H	3.508293168	-0.3265468145	-0.9555773598
H	2.3620098679	-1.5835601629	-1.3557625925
H	4.0238130144	-1.4768156717	1.2219373971
C	4.7423894526	-2.709410102	-0.4011211779
H	2.9411757855	-2.7850223415	0.7817071538
C	5.5425655295	-3.6828744142	0.4688477265
H	5.4154571118	-1.94669328	-0.8159332892
H	4.3235764028	-3.245605004	-1.2638007676
H	5.9970795514	-3.1661259273	1.3219106951
H	6.3471840432	-4.1622124869	-0.0981046315
H	4.8984641871	-4.4744045001	0.8687650586
H	4.8984641871	-4.4744045001	0.8687650586

TS endo 0353

E(RB3LYP) = -706.409737931 A.U.

First frequency = -529.9447 cm⁻¹

H	-0.7868604375	-0.6428311182	-2.103389715
C	-0.7083706117	-1.1216607827	-1.1342636337
H	0.0380115025	-1.9041723363	-1.09622188
C	-1.7942426228	-1.1588822144	-0.2634131772
C	-1.5747048227	-1.6914122501	1.0260977939
C	-0.3450884436	-2.1830055311	1.4315881261
H	-0.1996517769	-2.4689621513	2.4699151271
H	0.292372	-2.7121361844	0.7326204877
C	1.1523041393	-0.5345565894	1.142755238
H	0.7972475649	-0.0806548613	2.0658756467
C	2.4310965409	-1.3437159583	1.3151054711
C	0.7931160245	0.1305256514	-0.0347825803
H	1.4421658683	0.0346728112	-0.8999904292
C	0.0337000932	1.4334540097	0.0663719114
C	-3.1611259748	-0.5223411869	-0.5946592167
H	-2.3337241821	-1.5311365015	1.788193973
C	-4.216492426	-1.6545803568	-0.5567905798
C	-3.188279125	0.1118909311	-1.9969331433
C	-3.5652653025	0.5673866336	0.4247318927
H	-4.5724207176	0.9369417368	0.200704045

H	-2.8799846468	1.4181708273	0.3848942071
H	-3.5752569025	0.1902976216	1.4509219637
H	-4.18338747	0.5212543322	-2.1997269139
H	-2.9649096815	-0.6218422015	-2.7777927313
H	-2.4697433134	0.9336164891	-2.0833823559
H	-4.2706811307	-2.1167855567	0.4335022409
H	-3.9694840741	-2.4401176112	-1.2782579108
H	-5.2105712236	-1.2628087508	-0.8021001874
H	-0.7635105688	1.3154683767	0.8103436247
H	-0.4598542305	1.6691727149	-0.8842077098
C	0.9273939565	2.6173230349	0.4744704944
H	1.4085108173	2.3915369135	1.4357000599
C	0.1579779853	3.9386798815	0.5813082265
H	1.743554729	2.7266903548	-0.2539886431
H	-0.6587635378	3.8211742073	1.3068466409
H	-0.3224477126	4.1564145681	-0.3824506961
C	1.0451613421	5.1173832627	0.9916105266
H	0.472898347	6.0482515638	1.0620115512
H	1.850968384	5.2748037745	0.2654906824
H	1.5119330983	4.9376090812	1.9668530279
C	3.06671779	-1.9084415707	0.0291495596
H	2.2478463372	-2.1639296557	2.019491582
H	3.1722145127	-0.7011156211	1.8152498171
H	3.6079268336	-2.8324278348	0.2687504367
C	4.0454978191	-0.945564678	-0.659956925
H	2.2813221861	-2.2032069644	-0.6797342083
C	4.5645327888	-1.4814411226	-1.996417921
H	4.8893797768	-0.7604596828	0.0182622559
H	3.5671984983	0.0290704789	-0.8119760386
H	3.7424202526	-1.6290018225	-2.7064271688
H	5.0638793425	-2.4486538475	-1.8668417067
H	5.2824269039	-0.7941740217	-2.4556461338
H	5.2824269039	-0.7941740217	-2.4556461338

TS endo 0359

E(RB3LYP) = -706.411533370 A.U.

First frequency = -522.8431 cm^{-1}

H	-1.4117686401	0.1397587995	-1.9877473665
C	-1.0947517127	-0.5537407662	-1.2179941879
H	-0.2803637254	-1.1985246286	-1.520679212
C	-1.9568976034	-0.9382007202	-0.1983772597
C	-1.4363198373	-1.7538812041	0.8324248043
C	-0.1419973171	-2.2539387325	0.8105898797
H	0.2292635569	-2.8011768307	1.6732077532
H	0.2905435034	-2.5729244914	-0.131359138
C	1.2546649349	-0.5708328771	0.6677038669
H	1.2540264195	-0.4948121735	1.753582677
C	2.4561924819	-1.273628189	0.0702255649
C	0.6345055549	0.4688231928	-0.0275694279
H	1.0328008702	0.7292972117	-1.0045838613
C	-0.0892413826	1.5415306927	0.7465211472
C	-3.4083412406	-0.420585803	-0.0802090878
H	-2.0058915045	-1.8486606531	1.7541855593
C	-3.6045678581	0.476277798	1.1627592648
C	-4.3375997167	-1.6532719724	0.0425682787
C	-3.8532861286	0.3721993402	-1.3233321277
H	-3.2774469621	1.2930149504	-1.4543030799
H	-4.9053117583	0.6589902799	-1.2223688188
H	-3.7536866152	-0.2247474538	-2.2353518947
H	-4.1189685319	-2.2395138625	0.9395119025
H	-4.2231881958	-2.3136338475	-0.8230686554
H	-5.3856498978	-1.3368616443	0.0964336231
H	-3.2932307086	-0.028060386	2.0820367909
H	-4.6613745695	0.7454231576	1.2730909201
H	-3.0318390899	1.4033802271	1.0758609083
H	0.6139374551	1.9920071009	1.4621217372
H	-0.8533856115	1.0547518225	1.3671671229
C	-0.730477035	2.6570332803	-0.0882660671
H	-1.5295011017	2.2304458735	-0.7030936224
C	0.2360186437	3.4278669977	-1.004195901
H	-1.211777673	3.3685359688	0.5963482291
H	-0.3288991615	4.2173773413	-1.5158774591
H	0.6023457684	2.7643784872	-1.7980003705
C	1.4311222586	4.0497923122	-0.2740626529
H	2.0356961146	4.6599655182	-0.9529080425

H	2.0859405844	3.2814011654	0.1498716617
H	1.099646946	4.6938193207	0.5489512695
C	3.7443487693	-0.4374423883	0.1871320449
H	2.2656613522	-1.4825350604	-0.9931229679
H	2.6043227638	-2.2460435325	0.5535340214
H	3.5675373608	0.5382870893	-0.2828299742
C	4.9820745554	-1.0907912613	-0.4469523423
H	3.9433822899	-0.2324907735	1.2486328963
C	5.4339324375	-2.3837060311	0.2420542699
H	5.8083214103	-0.3686665608	-0.4280649421
H	4.778723062	-1.2926240211	-1.5078038924
H	4.6776712511	-3.171559242	0.1670608038
H	5.6282351577	-2.2120681883	1.3073104308
H	6.3548458775	-2.7702255272	-0.2065867143
H	6.3548458775	-2.7702255272	-0.2065867143

TS endo 0360

E(RB3LYP) = -706.410517459 A.U.

First frequency = -530.7754 cm^{-1}

H	-1.2774045372	-0.7571207517	-2.1748093074
C	-0.9130991753	-1.0306467004	-1.1913685159
H	-0.0355283518	-1.6627355338	-1.2143110816
C	-1.7723893877	-1.0747113136	-0.0965567288
C	-1.2009026871	-1.3223328344	1.1706614944
C	0.15486654	-1.5390486631	1.3521198476
H	0.5558482124	-1.5970326198	2.3605195015
H	0.7255145195	-2.0931373342	0.6165183312
C	1.2065734227	0.238180946	0.475702583
H	0.9694597579	0.7829338687	1.3853741417
C	2.6225103721	-0.3171558183	0.4474020751
C	0.510062908	0.6278455244	-0.673908946
H	0.9926633905	0.4697624267	-1.63600105
C	-0.4362915208	1.807984821	-0.6275170831
C	-3.2713394248	-0.7170369409	-0.1874343746
H	-1.8067029521	-1.1374232387	2.0547532229
C	-3.7104315608	-0.3896636813	-1.6259621251
C	-3.6368485468	0.4902617639	0.7064112764

C	-4.0732802861	-1.9521689592	0.2899891724
H	-3.8328072295	-2.2100103589	1.32571854
H	-3.8487541268	-2.8250577711	-0.3315293383
H	-5.1505265537	-1.7572043737	0.2321439007
H	-4.7172089262	0.6716783509	0.6723260815
H	-3.1329425183	1.3985384405	0.3658892259
H	-3.3643423203	0.3262080694	1.752533307
H	-3.5203224754	-1.225278837	-2.3069367751
H	-3.1951892936	0.4939623887	-2.0166831152
H	-4.7849186153	-0.1799011019	-1.6472402536
H	-0.9619495324	1.8046564571	0.3334553315
H	-1.2084435579	1.7065791004	-1.39801093
C	0.2665164891	3.1679444766	-0.841757033
H	0.7820162373	3.1416606793	-1.811440216
C	1.269115651	3.5877082071	0.2440024055
H	-0.5062901614	3.9449153882	-0.9285681326
H	1.7674441381	4.5096243098	-0.0820929881
H	2.0560082528	2.8287847859	0.3279513148
C	0.6344676235	3.8254042774	1.6184957382
H	1.3774584968	4.1738524059	2.343361605
H	0.1838915348	2.9135710296	2.0232682399
H	-0.1562336066	4.5826376708	1.5599751123
C	3.000483774	-1.1494232527	-0.7859355321
H	2.7937139289	-0.9089967464	1.353967683
H	3.3255672208	0.5285140174	0.515887851
H	2.2836560046	-1.9710215262	-0.9198658457
C	4.4203687045	-1.7353426829	-0.7246764051
H	2.9165470761	-0.5244402937	-1.6828805712
C	4.6078317838	-2.8165434059	0.3461175516
H	5.1391410416	-0.9215890102	-0.5563613469
H	4.6671191136	-2.1607440781	-1.705540088
H	3.8939264332	-3.6361006474	0.2024522828
H	4.4588326599	-2.4228237141	1.3564254302
H	5.6159125623	-3.241686001	0.3058330951
H	5.6159125623	-3.241686001	0.3058330951

TS endo 0364

E(RB3LYP) = -706.410136357 A.U.

First frequency = $-518.8728 \text{ cm}^{-1}$

H	-1.790826363	-0.0141555627	-2.1347960305
C	-1.2842643348	-0.5859260322	-1.3658395677
H	-0.4221451537	-1.1319835215	-1.730666554
C	-1.9735276058	-1.0412817897	-0.2449262906
C	-1.2206473268	-1.6804864549	0.7656619424
C	0.1364473362	-1.9302378324	0.6535010586
H	0.6734338801	-2.3249233387	1.5107418193
H	0.5712900852	-2.1878499041	-0.3049357041
C	1.144987699	0.0739912497	0.1835439913
H	1.2223779546	0.2239275051	1.2576435565
C	2.4049370067	-0.3916812561	-0.5172110156
C	0.2000954148	0.8364553799	-0.5047218673
H	0.4294061796	1.1024052973	-1.5337933211
C	-0.689141196	1.784788159	0.2642637234
C	-3.4735237588	-0.7615974342	-0.0107899462
H	-1.6834451749	-1.8281925768	1.7385822255
C	-4.0978899666	0.073973442	-1.1428398414
C	-3.7393602047	-0.0227674228	1.3208966255
C	-4.1916597266	-2.1327751656	0.032009798
H	-4.0374524503	-2.6813719749	-0.902797943
H	-5.2699382893	-1.9993438127	0.1785573765
H	-3.8129004157	-2.7540245304	0.8493582289
H	-4.8182118818	0.0827800737	1.48170969
H	-3.3028944288	0.9794738738	1.3110127979
H	-3.3321213693	-0.5596259963	2.1818085704
H	-5.1638972313	0.2278398179	-0.9457704694
H	-4.0088053651	-0.4254539187	-2.1126474652
H	-3.6299166928	1.0609516116	-1.2213580105
H	-1.1561154695	1.2113075192	1.0739499429
H	-1.5054302643	2.1395247506	-0.3773176906
C	0.0162128716	3.0040310534	0.8973016419
H	-0.7270923647	3.5201292925	1.5197285054
C	0.6229537851	4.0249905523	-0.0817805016
H	0.7985965893	2.6537532056	1.5839678545
H	0.7515730439	4.9765834479	0.4500851313
H	-0.0979234529	4.2267798397	-0.8864507605

C	1.9767666917	3.6294551029	-0.6858413618
H	2.7019498897	3.4013569652	0.1039327785
H	2.3886083814	4.4438217613	-1.2916921671
H	1.9031471563	2.7453579609	-1.323243186
C	3.363263012	-1.2179278718	0.3470747043
H	2.9485248898	0.4926070857	-0.8846456279
H	2.1381018428	-0.9605878821	-1.421680798
H	3.5956406603	-0.6541565833	1.2618954633
C	4.6683268171	-1.5729131773	-0.3735039008
H	2.872541175	-2.141494357	0.6764112909
C	5.6241151274	-2.397257217	0.4934854387
H	5.1671891919	-0.6490186477	-0.6965607434
H	4.433414864	-2.1277894435	-1.2922393346
H	6.5480450754	-2.6382764122	-0.04212358
H	5.1609023142	-3.3415253683	0.8019247732
H	5.8983945585	-1.8524970109	1.4041691084
H	5.8983945585	-1.8524970109	1.4041691084

TS endo 0365

E(RB3LYP) = -706.410174160 A.U.

First frequency = -542.4174 cm^{-1}

H	-1.5248543616	-1.2099686679	-1.953433622
C	-1.1209226369	-1.3151971969	-0.9529232072
H	-0.446169851	-2.1563579548	-0.848052957
C	-1.8352398875	-0.8588809623	0.1543734236
C	-1.1989693488	-0.9330660294	1.4126855618
C	0.0609550716	-1.4825260877	1.5813529097
H	0.557367396	-1.399743881	2.544519836
H	0.358784939	-2.3477187211	1.001295665
C	1.4434369416	-0.417982126	0.1426709759
H	1.6090965014	0.3394071991	0.9010013166
C	2.5179399358	-1.4808861643	0.0487803917
C	0.7132825544	-0.0650347056	-0.9974708029
H	0.9713078264	-0.6022733661	-1.9094639168
C	0.2057241339	1.3483197532	-1.2454254915
C	-3.2220424411	-0.1901633298	0.0424481462
H	-1.6258505547	-0.3723421478	2.2412148612

C	-3.2436373487	1.2337172417	0.6411523387
C	-4.2196710541	-1.0753164998	0.8293818991
C	-3.7125993633	-0.0928226717	-1.4134673808
H	-3.0496666907	0.5290477374	-2.024584378
H	-4.7078512611	0.3629642421	-1.4394399312
H	-3.7859854553	-1.0783165071	-1.8838450302
H	-4.2397094247	-2.0924809761	0.4250381741
H	-5.2329742622	-0.6611204003	0.7689437573
H	-3.9437496234	-1.1421814748	1.8860825454
H	-2.612420101	1.9106549188	0.0617919501
H	-2.8973000764	1.2538411556	1.6779869914
H	-4.2640302082	1.6331627772	0.6280822585
H	-0.7931717651	1.3166091858	-1.6971757525
H	0.8559690589	1.8082433313	-2.0061439541
C	0.166728805	2.2726866577	-0.0234915726
H	-0.4216163054	1.8026129143	0.7729103728
C	-0.4053422997	3.6574109515	-0.3454477983
H	1.1807984922	2.3977604372	0.377810684
H	-1.3982510441	3.5493296881	-0.8026901231
H	0.2231257057	4.1392246861	-1.106948837
C	-0.5081418245	4.5577090601	0.8884878037
H	-1.1681448644	4.112606551	1.6418526136
H	-0.9069254635	5.5456600981	0.6362875706
H	0.473401464	4.7020905123	1.3543350117
C	3.8181736781	-0.9469882646	-0.5819403292
H	2.1525702685	-2.3227170157	-0.5587411847
H	2.7342771614	-1.8884448992	1.0426619811
H	3.5786787372	-0.5253484611	-1.5662210811
C	4.9252250692	-2.0015799502	-0.7356600816
H	4.192818483	-0.1103081669	0.024654733
C	5.4690275461	-2.5412967404	0.592301268
H	5.7522324855	-1.5613766605	-1.3073725995
H	4.5460531795	-2.8356025842	-1.3424325612
H	5.839077292	-1.7252258377	1.224032154
H	6.2981760928	-3.2369927446	0.427016191
H	4.7011930612	-3.0762522686	1.1601714211
H	4.7011930612	-3.0762522686	1.1601714211

TS endo 0383

E(RB3LYP) = -706.409293139 A.U.

First frequency = -528.9463 cm^{-1}

H	-0.9968834793	-0.9028916219	-2.0545379903
C	-0.8622052469	-1.237833012	-1.032566585
H	-0.0556229474	-1.9495273648	-0.9123607458
C	-1.92584803	-1.2421111166	-0.1338985648
C	-1.6408323618	-1.5792215306	1.2071792873
C	-0.366470288	-1.9051453908	1.6392035915
H	-0.1790077196	-2.034457387	2.7018246643
H	0.3049006433	-2.4662284274	0.9991918143
C	0.9598798604	-0.181568084	1.0911275994
H	0.5636773365	0.3758479903	1.9364888953
C	2.3071996744	-0.836019263	1.3732497361
C	0.555159981	0.2677091844	-0.172150563
H	1.2098715787	0.070501168	-1.0165196254
C	-0.2614351769	1.5368977057	-0.2967589192
C	-3.341195545	-0.7475657394	-0.5000276994
H	-2.3966666334	-1.378344082	1.9628885719
C	-3.4585040972	-0.3491335805	-1.9822368068
C	-3.7672925749	0.468138277	0.3545298513
C	-4.3254314323	-1.9131131756	-0.2372780344
H	-4.0606179368	-2.7885262475	-0.8390661923
H	-5.3491319466	-1.6167288291	-0.494066811
H	-4.3167000368	-2.2164752553	0.8138401465
H	-3.1252053921	1.3306403758	0.1577293868
H	-3.7233724044	0.2535076806	1.4257604701
H	-4.7984691317	0.7541630441	0.1174992793
H	-2.805471561	0.4942503437	-2.2296229676
H	-4.486546378	-0.0445237387	-2.2043003134
H	-3.2066527201	-1.1823741175	-2.6459084682
H	-0.943404054	1.607699919	0.5595239222
H	-0.8905057374	1.5030688631	-1.1929498048
C	0.6035594916	2.813528439	-0.367031401
H	1.2777709246	2.7409463394	-1.2328430298
C	1.431168369	3.1119961686	0.8880668033
H	-0.0567065323	3.6686425286	-0.5696567934

H	2.1274790222	2.2859320693	1.0727850918
H	0.7637048739	3.1476178591	1.7602233916
C	2.2117718482	4.4251932087	0.7808206653
H	2.7985256892	4.6198884609	1.6845905246
H	1.5377751626	5.2764361378	0.6303650194
H	2.9053294637	4.4014208195	-0.0677852856
C	3.0154847744	-1.4977865919	0.1751975427
H	2.1948996073	-1.5699207468	2.1799627411
H	2.9753993826	-0.0637523887	1.7855491832
H	3.6466862676	-2.3191850402	0.5369808633
C	3.8983867657	-0.5367354961	-0.6354632672
H	2.2750044764	-1.9660049436	-0.4875075834
C	4.4910680096	-1.1863190848	-1.8882042066
H	4.7076951733	-0.175173625	0.0131129655
H	3.3229855738	0.3530241114	-0.9169659945
H	5.0869697089	-2.0695992573	-1.6306658886
H	5.1399065834	-0.4934905844	-2.433714184
H	3.6999072167	-1.5124280254	-2.5733755719
H	3.6999072167	-1.5124280254	-2.5733755719

TS endo 0386

E(RB3LYP) = -706.411361355 A.U.

First frequency = -512.7883 cm^{-1}

H	-1.8628882064	0.1739786129	-2.0010461985
C	-1.3556424115	-0.5448733103	-1.3679396173
H	-0.6597869401	-1.1783812274	-1.9055027233
C	-1.9453288325	-1.0002899315	-0.1919050743
C	-1.176910925	-1.8523517365	0.6344043222
C	0.0872595815	-2.2974046489	0.294745307
H	0.6685027693	-2.8571960068	1.0212399991
H	0.3423602311	-2.5004752865	-0.7381529113
C	1.334555268	-0.4027008456	-0.1527251942
H	1.5444308221	-0.3646088655	0.9116367618
C	2.4138881462	-0.9838732767	-1.0440726943
C	0.4418714777	0.5444154531	-0.6539833453
H	0.5882898594	0.8663539026	-1.6837768552
C	-0.1582309577	1.5622418837	0.2877679453

C	-3.3240657857	-0.5116699333	0.300571453
H	-1.5173437167	-2.0265164099	1.6525196868
C	-3.2549626018	0.1375693472	1.7019468829
C	-4.2503193592	-1.7504086079	0.3729823645
C	-3.9617015072	0.5093639018	-0.6589492642
H	-3.3543319839	1.4163482151	-0.746862595
H	-4.9463409567	0.806518232	-0.2833693838
H	-4.1008797431	0.0920942278	-1.6611914971
H	-4.3351242131	-2.2299438351	-0.6075562762
H	-5.2552722158	-1.4616794583	0.7025429096
H	-3.8648145578	-2.4951903898	1.0758737838
H	-2.8184236211	-0.5321470506	2.4477693921
H	-4.2627757729	0.3974285246	2.0451602859
H	-2.6605026373	1.0546613508	1.6832157741
H	-0.5271756431	1.032955419	1.1735661321
H	-1.0305857667	2.0395129184	-0.1717953357
C	0.8466789327	2.6414370118	0.7438988858
H	0.329165588	3.3415003911	1.414936072
C	1.5061625675	3.4309659236	-0.3977498493
H	1.6326197035	2.1603723092	1.3402021901
H	2.1135872526	2.7474159472	-1.0047987192
H	2.2063787252	4.1561523265	0.0358218042
C	0.5111137623	4.1667464515	-1.3015667859
H	-0.1321206454	4.8353854975	-0.7174085528
H	-0.1409265177	3.4681156258	-1.8365085963
H	1.0289753925	4.7729054424	-2.0519380728
C	3.2908191777	-2.0870826269	-0.4263630709
H	3.0688544669	-0.1637733282	-1.3718797809
H	1.9552389475	-1.365738626	-1.9682306462
H	2.7013018555	-3.0005658628	-0.2901426376
C	3.9509725551	-1.7191791487	0.9134651607
H	4.0777466113	-2.337690205	-1.1502901615
C	4.7743636901	-0.4273599699	0.8707179006
H	4.595460708	-2.5522523581	1.2211671912
H	3.1830809241	-1.6347055191	1.6928160637
H	4.1411235841	0.445184064	0.6790027341
H	5.5319614903	-0.4676267223	0.0792517819
H	5.2922091352	-0.2565379752	1.8199812445

H 5.2922091352 -0.2565379752 1.8199812445

TS endo 0388

E(RB3LYP) = -706.409087649 A.U.

First frequency = -542.1485 cm⁻¹

H -1.6350412379 -1.5236830908 -1.8993220678
C -1.295036386 -1.525408482 -0.8699718912
H -0.5791114781 -2.309193154 -0.6533446479
C -2.1015775317 -1.0205651011 0.1483730492
C -1.5465725441 -0.9544855391 1.4443611402
C -0.2679879951 -1.4041198136 1.7316132126
H 0.1570025317 -1.2159477574 2.7140653679
H 0.1188705088 -2.2919257891 1.2452415709
C 1.1118883531 -0.345269388 0.3192235868
H 1.1554094174 0.4792558196 1.02160481
C 2.2816140676 -1.3049345663 0.3898972905
C 0.4571857944 -0.1426084957 -0.9016360491
H 0.8286098574 -0.736355473 -1.7359558592
C -0.1486255392 1.1935063811 -1.3237602121
C -3.496041223 -0.4095815131 -0.1058289794
H -2.0568600233 -0.3558817175 2.1955291751
C -3.5686310038 1.0724529206 0.3267442361
C -4.5177912442 -1.2224826273 0.7260032858
C -3.9133058696 -0.4914722719 -1.5853086028
H -3.2427949088 0.0850280655 -2.2314425642
H -4.9209478122 -0.0813596375 -1.7094823181
H -3.9272070595 -1.5252118574 -1.9448765596
H -4.5030129454 -2.278089773 0.4360380099
H -5.5326993411 -0.8378773936 0.5714400106
H -4.2958765729 -1.1678141438 1.7959388395
H -3.2976393988 1.2093841664 1.3770505721
H -4.5877934521 1.4541843503 0.1970503173
H -2.8984089003 1.6918772448 -0.273832911
H -1.1616129986 1.0357034265 -1.7060858025
H 0.4307883228 1.5628638878 -2.1836271026
C -0.181659547 2.3020558762 -0.2570288958
H -0.9415543653 3.0426866414 -0.5387181851

C	1.1549092521	3.0361499012	-0.0761689946
H	-0.5187670113	1.885231507	0.7003315479
H	1.4030723811	3.5489569172	-1.0154157949
H	1.9607027512	2.3117101733	0.089587493
C	1.1248980783	4.0474604508	1.0725618016
H	0.9254439591	3.5493327367	2.0285718253
H	0.3364421101	4.7939492087	0.9214849984
H	2.0762553793	4.5812220255	1.1667163143
C	3.5804907976	-0.6926249725	-0.1633162389
H	2.0463905446	-2.2154462085	-0.1809841073
H	2.4552307125	-1.6270550136	1.4246516235
H	3.4176791633	-0.3884581451	-1.2059544325
C	4.7811543381	-1.6418526011	-0.0836294182
H	3.806967804	0.2304597566	0.3890745876
C	6.0681231765	-1.0241663723	-0.6380063033
H	4.5483643174	-2.5644646084	-0.6329358678
H	4.9365616023	-1.9422683621	0.9615734123
H	6.9107898875	-1.7201057136	-0.5716171842
H	6.3393027378	-0.1174597688	-0.085183519
H	5.9483435741	-0.7439076362	-1.6907833389
H	5.9483435741	-0.7439076362	-1.6907833389

TS endo 0398

E(RB3LYP) = -706.410369719 A.U.

First frequency = -506.6874 cm^{-1}

H	-1.4631824062	-0.4308898941	-2.27635189
C	-1.0153254592	-0.8614929469	-1.3854545452
H	-0.1720806123	-1.5084165488	-1.5936518535
C	-1.7786174262	-1.0407718692	-0.2350211333
C	-1.1166380078	-1.5060007101	0.9244596172
C	0.2138305643	-1.8839199637	0.9333107701
H	0.6875913366	-2.1299294812	1.8785953046
H	0.6596056471	-2.3603809768	0.0684100977
C	1.4210586202	-0.0855973398	0.1346274411
H	1.4676831666	0.244437621	1.1694666276
C	2.6480820405	-0.7952380469	-0.4026702398
C	0.5733063997	0.6080608805	-0.7254096278

H	0.8637217621	0.6644798116	-1.7733230199
C	-0.2542473092	1.7549102965	-0.1994860516
C	-3.2761608408	-0.66133278	-0.217955106
H	-1.6130957424	-1.405717695	1.8841818081
C	-4.022387948	-1.7182284309	-1.0697699549
C	-3.541976484	0.7348545002	-0.8206782137
C	-3.8767971622	-0.6781182091	1.2005191836
H	-3.8023398832	-1.6667697074	1.6639677743
H	-4.938961019	-0.4163378418	1.1547428945
H	-3.3840414338	0.0472129616	1.8565845144
H	-3.1351701164	0.8367555794	-1.8304693986
H	-3.1078361645	1.5221194312	-0.1995916517
H	-4.6212264016	0.9128934243	-0.8846500063
H	-3.6689807172	-1.7072514128	-2.1054308561
H	-5.1013143037	-1.5225603352	-1.0743285054
H	-3.8584104918	-2.7248433261	-0.6714571959
H	-0.8041309749	1.4117534099	0.6880110654
H	-1.0066977401	2.0447310239	-0.9397124369
C	0.5805068247	2.9929342047	0.1736975251
H	1.3284968569	2.7150016442	0.9280131757
C	-0.2755518543	4.1498602692	0.7011178745
H	1.1483203304	3.3292404613	-0.7052732363
H	-0.844854069	3.806072462	1.5757707076
H	-1.0220125444	4.42262907	-0.0574740081
C	0.5500566024	5.3835737096	1.0768329169
H	1.104050978	5.7648119828	0.2113348729
H	1.2823557243	5.1444670945	1.8565180856
H	-0.083199789	6.1946180943	1.4512321474
C	3.4999188499	-1.499902574	0.6609042493
H	3.2846357917	-0.0610741824	-0.9204344217
H	2.3426586623	-1.5099731181	-1.1806914207
H	3.7275326447	-0.7780672123	1.4569243067
C	4.8148159497	-2.0833900075	0.1224016824
H	2.920342494	-2.3022842632	1.1330238608
C	4.6233688458	-3.218214516	-0.8907039292
H	5.4076555603	-2.4551307321	0.9676865428
H	5.4075217863	-1.2795114447	-0.3355552598
H	5.5846575176	-3.6463139868	-1.1927990341

H	4.1189673537	-2.8722444048	-1.7985876739
H	4.0175720387	-4.0260298982	-0.4633999339
H	4.0175720387	-4.0260298982	-0.4633999339

TS endo 0401

E(RB3LYP) = -706.410115002 A.U.

First frequency = -519.0935 cm⁻¹

H	-1.1357805327	-0.3038534325	-2.0715559051
C	-0.8782207619	-0.7992930124	-1.1428975104
H	0.0342979424	-1.3771382244	-1.1956678732
C	-1.8540941906	-1.1199523042	-0.205256305
C	-1.4233665137	-1.6483310738	1.0327867856
C	-0.0892104347	-1.8792907217	1.327313218
H	0.1904694353	-2.1734456359	2.3354022849
H	0.586497562	-2.2355882086	0.5589457134
C	0.990738163	0.0576516618	1.0483688324
H	0.6403352027	0.3643567551	2.0315380492
C	2.4247717979	-0.4452598936	1.0400590695
C	0.4064658398	0.7142781134	-0.0374475795
H	0.9795013557	0.804957755	-0.9545444788
C	-0.6216243759	1.791599633	0.2202711004
C	-3.3511959119	-0.8029992931	-0.4115758606
H	-2.1376684165	-1.6942178906	1.8512056561
C	-3.619369438	-0.0833548938	-1.7456253907
C	-3.9342982922	0.0726800262	0.7210271463
C	-4.1050336668	-2.155300694	-0.4298746975
H	-3.728627899	-2.7989183576	-1.2315389801
H	-5.1778509097	-1.9970529474	-0.5910438433
H	-3.9800766634	-2.6925124503	0.5152866302
H	-3.7969286172	-0.3783094393	1.707352146
H	-5.0111310578	0.2106505095	0.5715374127
H	-3.4695487451	1.0622801437	0.7351066645
H	-3.1105710036	0.8852992984	-1.7907654671
H	-4.6928060215	0.1006730679	-1.8586865401
H	-3.2936573199	-0.6817301714	-2.6021757224
H	-1.3720182814	1.3812875416	0.9063138697
H	-1.1500348407	2.0384278862	-0.7089582066

C	-0.0723713008	3.0946657106	0.8414606145
H	-0.9337534993	3.7444332627	1.0461802388
C	0.9416968515	3.8753312341	-0.0162990932
H	0.3784244886	2.8690405872	1.8173754046
H	0.9260046544	4.9271258218	0.2968182671
H	0.6091393252	3.8701479354	-1.0637966756
C	2.3893701263	3.3736931056	0.0713611123
H	2.739008774	3.383383779	1.110309512
H	3.0625796555	4.0111047225	-0.5120986361
H	2.494880932	2.3503729728	-0.2960415397
C	2.9657296953	-0.9416670127	-0.3065702463
H	2.5405948032	-1.2451370344	1.7834528008
H	3.0722334975	0.3745310362	1.3893452962
H	2.3166479453	-1.7325134497	-0.7064676897
C	4.3996287258	-1.4745586309	-0.2085430903
H	2.9398603781	-0.1286528408	-1.0436666438
C	4.9508965618	-1.9541964874	-1.5540615057
H	4.4306299511	-2.297919245	0.5178095192
H	5.0491346091	-0.6869508112	0.1970634766
H	5.9744798325	-2.3306045684	-1.4587107249
H	4.9613608013	-1.1404024664	-2.288169344
H	4.3352610576	-2.761775039	-1.9665829175
H	4.3352610576	-2.761775039	-1.9665829175

TS endo 0409

E(RB3LYP) = -706.411251679 A.U.

First frequency = -539.7937 cm⁻¹

H	-1.2765969161	0.4798896963	-1.9401999579
C	-0.8794072821	-0.2464861643	-1.2407711334
H	-0.0369550163	-0.8048617757	-1.6295172959
C	-1.6815427341	-0.7885766785	-0.2416313162
C	-1.0655351625	-1.6419486447	0.7009485454
C	0.2575929477	-2.0470111299	0.5990288367
H	0.6903473027	-2.6310327976	1.4060659851
H	0.6786858322	-2.2592359899	-0.3774002045
C	1.5514094491	-0.2336160946	0.477899729
H	1.656073805	-0.287267275	1.5595028847

C	2.7271052654	-0.7566443287	-0.3267342392
C	0.7645852983	0.8023463197	-0.0280149466
H	1.0567616897	1.2426286628	-0.9782265708
C	-0.0111712778	1.6673764206	0.9347925905
C	-3.1669416127	-0.4089162006	-0.0501404213
H	-1.5963270832	-1.8602026337	1.6250038655
C	-3.4157137272	0.3180097982	1.2906365163
C	-3.987354505	-1.7224873684	-0.0637432988
C	-3.6985322749	0.4837062142	-1.1866891271
H	-3.1986096405	1.4563472492	-1.2143944538
H	-4.7674069857	0.6714879098	-1.0402699681
H	-3.5730014692	0.0066666006	-2.1637943059
H	-3.6996746042	-2.3876801096	0.755440274
H	-3.8358555879	-2.2652846984	-1.0023364283
H	-5.0570777362	-1.5062000981	0.0386703765
H	-2.9213167154	1.2925864707	1.3095392792
H	-3.0522827458	-0.2620161431	2.1436331049
H	-4.4890915014	0.4848024259	1.4368913729
H	0.6827176217	2.0741211414	1.6867630549
H	-0.6951004354	1.0151848055	1.4944202216
C	-0.7804135124	2.8314862496	0.3011923045
H	-1.435332975	2.445529699	-0.4882578917
C	0.1157980514	3.9316414424	-0.2824716435
H	-1.4403743461	3.2806123094	1.0556208627
H	0.7858736762	3.5034517776	-1.0388083674
H	0.7666282998	4.323934423	0.510849454
C	-0.6865256321	5.076653796	-0.9070391011
H	-1.3207875433	4.7120973202	-1.7233765939
H	-0.0318699019	5.8538451122	-1.3146386665
H	-1.343286701	5.5473463158	-0.1663707665
C	3.5450806976	-1.8548657048	0.3616698069
H	3.4003234676	0.0830483743	-0.5558897731
H	2.3757755148	-1.1181008826	-1.3059481387
H	3.8722535225	-1.4928213987	1.3468469819
C	4.7699333072	-2.2906471483	-0.4497250481
H	2.9134643708	-2.7301912813	0.5550131004
C	5.5864706554	-3.385362732	0.2428430634
H	5.4092107558	-1.4175246675	-0.6389448682

H	4.4411126465	-2.6451469913	-1.4362938472
H	6.4547779543	-3.6799959949	-0.3553501743
H	4.9788843421	-4.2815032194	0.4134155651
H	5.9527474051	-3.0456020244	1.218407173
H	5.9527474051	-3.0456020244	1.218407173

TS endo 0410

E(RB3LYP) = -706.410529323 A.U.

First frequency = -508.0015 cm⁻¹

H	-1.6644923329	-0.4557600959	-2.1439070577
C	-1.1509045278	-0.8628132338	-1.2776166661
H	-0.371557698	-1.5715222891	-1.5290150307
C	-1.7991542552	-0.9284548999	-0.0472081128
C	-1.0468455863	-1.3656122113	1.0669864447
C	0.2550895749	-1.8223454794	0.9658939929
H	0.8098321316	-2.0426617972	1.8727097314
H	0.5807597199	-2.3753335434	0.0929723076
C	1.4706554084	-0.1538575777	-0.0611002452
H	1.6438427423	0.2307734772	0.9409484562
C	2.5957389151	-0.9644842508	-0.6735743452
C	0.5773333778	0.5416999076	-0.8721118599
H	0.7586400864	0.5228182686	-1.9455957092
C	-0.1336318022	1.7595579743	-0.335619262
C	-3.2632305355	-0.45542973	0.0956461586
H	-1.4346701109	-1.1805271426	2.0634389098
C	-3.5064729018	0.9280291931	-0.5455504609
C	-3.7197340323	-0.3740134789	1.5646283862
C	-4.151304369	-1.4985328776	-0.6273179191
H	-4.0069639539	-2.4955649224	-0.1984898389
H	-3.9038729887	-1.5539767343	-1.6918578658
H	-5.2120136223	-1.2360384419	-0.5360188729
H	-3.1257824461	0.3495030417	2.1330051983
H	-3.6527331237	-1.343954691	2.0671303708
H	-4.7654150843	-0.0524412067	1.6089129789
H	-4.5751263802	1.1682909719	-0.5180143447
H	-3.1915250907	0.9632759505	-1.592056822
H	-2.9721730354	1.7126668521	-0.003966903

H	-0.5958294586	1.4987676754	0.6271236938
H	-0.948405126	2.0341902018	-1.0093993224
C	0.7950173286	2.9714342532	-0.132001274
H	1.6365030201	2.6716588691	0.5048102082
C	0.094298842	4.1874291558	0.4940830169
H	1.2320173681	3.25941683	-1.098730408
H	0.8449736726	4.9625181538	0.6951179701
H	-0.3163930065	3.8995929551	1.4718945617
C	-1.0221082406	4.7852861285	-0.3704017145
H	-0.6461558558	5.0546113732	-1.3645456605
H	-1.4345612031	5.6908080695	0.0865002793
H	-1.8499747335	4.0826766187	-0.5101004842
C	3.5159367587	-1.6611185157	0.3345174647
H	3.2101713484	-0.2996006774	-1.2995178716
H	2.1803626653	-1.7097172361	-1.3700937125
H	3.902095948	-0.9136668932	1.0422670891
C	4.6924320318	-2.3873859969	-0.3263918004
H	2.9426641143	-2.3782798334	0.9339454437
C	5.6099370723	-3.081109556	0.684393422
H	5.274269529	-1.6697071664	-0.9207179479
H	4.3043319366	-3.1274797108	-1.0396857194
H	6.0349136485	-2.3587305982	1.3907200806
H	6.4417632091	-3.5924130207	0.1891704218
H	5.0593960915	-3.8274815686	1.2684851668
H	5.0593960915	-3.8274815686	1.2684851668

TS endo 0413

E(RB3LYP) = -706.410745238 A.U.

First frequency = -526.0435 cm^{-1}

H	-1.3847693732	0.3418681686	-1.9131967911
C	-1.1273796482	-0.5091506641	-1.2937925652
H	-0.5002771873	-1.2353928932	-1.7951515281
C	-1.9414023148	-0.8950184041	-0.2341242795
C	-1.4849600872	-1.9443020035	0.5951873803
C	-0.325220659	-2.6593395455	0.3308568392
H	0.0234856986	-3.390192507	1.0558698635
H	-0.0660629912	-2.8984007652	-0.6943360723

C	1.3548179137	-1.2285598521	0.1968756536
H	1.4889869031	-1.3538336724	1.2674573349
C	2.2933113815	-2.0205533521	-0.6912997451
C	0.8518646781	0.0022225303	-0.228907705
H	1.1765864498	0.3756152693	-1.1967799246
C	0.4358480575	1.0161009565	0.8078645539
C	-3.2430108304	-0.1528055917	0.1436445576
H	-1.9624447388	-2.0836851451	1.5625690012
C	-3.1421965361	0.5329862724	1.5247641146
C	-4.381856913	-1.2011342715	0.189158377
C	-3.634029251	0.9152819458	-0.8944916269
H	-2.8987610749	1.7234438525	-0.9498068631
H	-4.5927546253	1.3664280917	-0.617883884
H	-3.7430387306	0.4825882432	-1.8939739505
H	-4.1982842189	-1.966290284	0.9488076343
H	-4.4822584386	-1.7076454277	-0.7761798604
H	-5.337143614	-0.7175517005	0.4238357519
H	-2.8504005997	-0.1702573913	2.3099662965
H	-4.1110351022	0.961323058	1.8063029076
H	-2.4106603512	1.3453284876	1.5095093596
H	1.2831494847	1.1954456862	1.488301416
H	-0.3439678409	0.5578880205	1.4301592213
C	-0.0371725968	2.365924745	0.2591513561
H	-0.8430913377	2.2018852026	-0.4653501717
C	1.0745256982	3.1921824108	-0.4014221425
H	-0.4740259567	2.9549007245	1.0768945797
H	1.5246720385	2.6202599906	-1.2228466592
H	1.8795523721	3.3579909983	0.3275818869
C	0.5741248018	4.5371567397	-0.9353700919
H	-0.20912524	4.3937868557	-1.6887136966
H	1.3812656022	5.113827779	-1.3987364795
H	0.1475371008	5.1464308516	-0.1302331451
C	3.6817083047	-1.3875675477	-0.9301794547
H	1.819431384	-2.1537663049	-1.6751105685
H	2.4303559917	-3.0295068033	-0.281528706
H	4.1977447615	-2.0083295473	-1.6748068274
C	4.5930713639	-1.2514712904	0.3028564931
H	3.5518348498	-0.3998705683	-1.392608084

C	4.27419496	-0.0719618363	1.2309979484
H	5.6266343473	-1.1391710205	-0.049196872
H	4.571949718	-2.1900660954	0.8741352718
H	3.3044346261	-0.1815438304	1.7209850214
H	4.2496516971	0.8692211929	0.6695722742
H	5.0342613827	0.0256337829	2.0136662362
H	5.0342613827	0.0256337829	2.0136662362

TS endo 0414

E(RB3LYP) = -706.409697697 A.U.

First frequency = -540.8066 cm^{-1}

H	-1.3655419448	-0.6325623677	-2.2344997357
C	-1.1114085537	-1.0535961948	-1.2683900031
H	-0.4528881699	-1.9114898908	-1.3327341226
C	-1.9818259884	-0.9293408531	-0.1863476981
C	-1.5352047187	-1.4082387833	1.064753524
C	-0.309952347	-2.0314270436	1.2322120704
H	0.0396936946	-2.2656679267	2.2341292699
H	0.0750024047	-2.6897417904	0.4626930928
C	1.2596202073	-0.6332670966	0.402221689
H	1.3090433233	-0.1481189428	1.3708461202
C	2.3433366698	-1.6574880625	0.1393025653
C	0.7047159773	0.0775969889	-0.6675562868
H	1.095974848	-0.172529896	-1.6530903108
C	0.2412063527	1.5230227167	-0.5474642675
C	-3.3396420541	-0.2015109467	-0.2799130324
H	-2.0816950587	-1.1103368113	1.9567673199
C	-4.4391119789	-1.2397017839	0.0531916866
C	-3.6143084434	0.3520638574	-1.6898062991
C	-3.4481321385	0.9739393998	0.7159353405
H	-2.7330357858	1.7613110615	0.4692456373
H	-3.2636257003	0.6627176734	1.7476342758
H	-4.4533163343	1.408994085	0.6790174351
H	-4.5969102726	0.8346362472	-1.7135865159
H	-3.6150593097	-0.4408937025	-2.4442008245
H	-2.8720020433	1.1021004938	-1.9831707579
H	-5.4335355177	-0.7832965971	-0.0161170992

H	-4.3183985263	-1.6356843202	1.0660178764
H	-4.3997747254	-2.084529667	-0.6419865702
H	-0.6891949523	1.6722623621	-1.1093838751
H	0.9928662653	2.145519649	-1.0539888377
C	0.0442718445	2.0472378513	0.8811179279
H	-0.638060729	1.3778413797	1.4161241653
C	-0.491567721	3.486149496	0.9426490306
H	1.0004007226	2.0082780024	1.4196033949
H	-0.7310084491	3.7274234016	1.9860262742
H	-1.4396018837	3.5501062121	0.3916677803
C	0.4798589319	4.5394723667	0.3964518638
H	1.4420530968	4.493412241	0.9199251509
H	0.0792162832	5.550515402	0.5230224142
H	0.6776185372	4.3967292431	-0.6706718238
C	3.7197296737	-1.0139613657	-0.1053254021
H	2.074056865	-2.2616374028	-0.7399693743
H	2.4245386644	-2.3580921611	0.9803013181
H	3.6486236361	-0.3298894346	-0.9616292355
C	4.8319273984	-2.03861716	-0.3548563306
H	3.984453259	-0.3893468515	0.7594333626
C	6.1971489717	-1.3899963445	-0.6011479631
H	4.559831677	-2.6637106615	-1.2164801245
H	4.8966904532	-2.719320153	0.504981184
H	6.9745187109	-2.140605946	-0.7776185057
H	6.5061932608	-0.7848137671	0.2587989397
H	6.1668085938	-0.7287287206	-1.4746896608
H	6.1668085938	-0.7287287206	-1.4746896608

TS endo 0416

E(RB3LYP) = -706.409984149 A.U.

First frequency = -508.7761 cm^{-1}

H	-1.5873991912	-0.4577456061	-2.2624557268
C	-1.1541042078	-0.908303493	-1.3741457947
H	-0.3549018501	-1.6069849053	-1.5891133842
C	-1.9131179974	-1.0355754748	-0.2135673611
C	-1.2659047327	-1.5318080051	0.9411234838
C	0.0395404765	-1.9890843752	0.9375754143

H	0.5075920049	-2.256359737	1.8799831677
H	0.4455813521	-2.4985004532	0.0719845089
C	1.3447164893	-0.2752977697	0.0992526799
H	1.4324796658	0.0528856853	1.1318641035
C	2.5138910031	-1.0628185419	-0.459243362
C	0.5231950192	0.4663286319	-0.7462711417
H	0.798490717	0.5061978207	-1.7990433617
C	-0.2247558273	1.660869853	-0.2073735036
C	-3.3851930317	-0.5678468304	-0.1816573679
H	-1.7440570861	-1.396082776	1.9057843206
C	-4.2026026153	-1.5821036568	-1.0198991981
C	-3.5746438051	0.8391704134	-0.7880105293
C	-3.9694906691	-0.543017421	1.2435016844
H	-3.9474725624	-1.5322304212	1.7112017135
H	-5.0150259832	-0.2198568274	1.2082091871
H	-3.427781356	0.1552836779	1.8902309755
H	-3.1747556154	0.9124076629	-1.8030233884
H	-3.0867757534	1.601578214	-0.1758663015
H	-4.6420456462	1.0810831958	-0.8399950203
H	-3.860699372	-1.5970804698	-2.059375107
H	-5.2678930203	-1.3222977426	-1.0139488374
H	-4.0947396957	-2.5949038038	-0.6181272591
H	-0.7781155922	1.3523550412	0.6906062294
H	-0.9715459746	1.9946929532	-0.9346151951
C	0.6898224656	2.846635925	0.1480325184
H	1.4331884107	2.5248066602	0.8893525918
C	-0.0848587945	4.0539063915	0.6882011604
H	1.2609704912	3.1469746715	-0.7417466926
H	-0.6582529608	3.7462423357	1.57356584
H	-0.8268121849	4.3708602424	-0.0575365286
C	0.8208473784	5.2354675691	1.0466201081
H	1.5510497528	4.9529829544	1.813660283
H	0.244897143	6.0839230913	1.430524271
H	1.3814732835	5.5814117763	0.1706290195
C	3.3645282606	-1.7758875368	0.5989113541
H	3.1532659825	-0.3763610186	-1.0309267531
H	2.1517131522	-1.7987225755	-1.1950113157
H	3.7407348319	-1.0293483459	1.3131337582

C	4.5483085442	-2.5704203927	0.0262646886
H	2.7289772565	-2.4560457385	1.1765545562
C	5.6186701601	-1.7081789306	-0.6531841107
H	4.1697224591	-3.314964745	-0.6877434978
H	5.0142397778	-3.1405115609	0.8399720457
H	6.0014350826	-0.9455206169	0.0351469489
H	5.2273528386	-1.1905613363	-1.5347001479
H	6.4672612606	-2.3173614028	-0.9810776967
H	6.4672612606	-2.3173614028	-0.9810776967

TS endo 0428

E(RB3LYP) = -706.410739273 A.U.

First frequency = -511.9232 cm^{-1}

H	-1.1212570573	-0.3006571144	-2.1096715762
C	-0.8616591609	-0.8178467355	-1.1910963142
H	0.0505944225	-1.393125826	-1.2566695887
C	-1.8455156779	-1.1482620948	-0.2653766147
C	-1.4305489581	-1.7105802132	0.963398865
C	-0.1048942614	-1.9988472111	1.2455743739
H	0.1669017408	-2.3267217696	2.2452091851
H	0.5547657533	-2.3597753983	0.4653217706
C	1.0514418892	-0.0958538842	1.043764214
H	0.7194598091	0.1653555877	2.0462185479
C	2.4622341841	-0.6602454428	0.9932943067
C	0.4798841475	0.6363445178	0.0030767763
H	1.0467438723	0.762774493	-0.9138734557
C	-0.5236550687	1.7186310538	0.3289713222
C	-3.3302066913	-0.8267926612	-0.5491330492
H	-2.1356073339	-1.7445888343	1.7873674194
C	-3.8154245693	-1.8352888612	-1.6198979944
C	-3.5337806271	0.6039831505	-1.0920048294
C	-4.2216926092	-0.9832879721	0.697460813
H	-3.9172237192	-0.3027360053	1.499641823
H	-4.2023186376	-2.0053666825	1.0882427252
H	-5.2603646747	-0.7510826647	0.4404185301
H	-3.2769268129	1.3532643355	-0.3393338914
H	-4.5838987836	0.7500594722	-1.3684016705

H	-2.9331182645	0.8009300729	-1.9840401343
H	-3.2448293484	-1.7252455784	-2.5472580345
H	-4.8761637072	-1.678741364	-1.8494339669
H	-3.6889845847	-2.865054964	-1.2699575933
H	-1.2933090267	1.2906184727	0.9847410204
H	-1.0342575761	2.0447697152	-0.5834081988
C	0.098233521	2.9474281844	1.0227790568
H	-0.7043428812	3.6503240882	1.2876209271
C	1.1434825818	3.6759690388	0.1704445576
H	0.560107565	2.6347999191	1.9691061512
H	0.689481974	3.9648537328	-0.7878753981
H	1.9569305429	2.98124524	-0.0750594998
C	1.7188734554	4.9143171994	0.8628799028
H	2.4637334951	5.4176292727	0.2376096844
H	2.203809874	4.6456147151	1.808507669
H	0.9304847328	5.6403183734	1.0928795154
C	2.9731570947	-1.0954011547	-0.3857448491
H	2.5443490703	-1.5102626851	1.6838108847
H	3.1488960025	0.1032345798	1.3912354979
H	2.286713358	-1.8300597829	-0.8280122216
C	4.3813730921	-1.6988206186	-0.3328287573
H	2.9796603305	-0.2372201686	-1.0699407805
C	4.9018954177	-2.119771724	-1.7098910193
H	4.3780963469	-2.5660016634	0.3413418216
H	5.0696050515	-0.9689233595	0.1147831501
H	5.9074124152	-2.5480612634	-1.6466021022
H	4.9458074345	-1.2638485468	-2.3930726799
H	4.2469887992	-2.8713211804	-2.1655623805
H	4.2469887992	-2.8713211804	-2.1655623805

TS endo 0445

E(RB3LYP) = -706.410205762 A.U.

First frequency = -507.5682 cm⁻¹

H	-1.9500451137	-0.4773325022	-2.2332284267
C	-1.3686727976	-0.918510128	-1.428980055
H	-0.6741210938	-1.6792996759	-1.7631902042
C	-1.8710969903	-0.938577042	-0.1306968338

C	-1.0258969459	-1.4288861237	0.8911265842
C	0.2200313959	-1.9763130159	0.6421443186
H	0.8600381064	-2.2361792809	1.4798452751
H	0.4025973166	-2.5497481174	-0.2586396654
C	1.4162711646	-0.390295797	-0.525209871
H	1.7165140777	-0.0197997216	0.4498522562
C	2.4061142394	-1.271296743	-1.2637679611
C	0.4855080771	0.365785738	-1.2339611529
H	0.5453098425	0.3408187643	-2.3209779581
C	-0.0774048959	1.6240929258	-0.6211046115
C	-3.2706145062	-0.3634061429	0.1819806561
H	-1.279872168	-1.2172633212	1.9246751157
C	-4.3083712643	-1.3678870733	-0.3779710924
C	-3.5111041862	1.0117827955	-0.4770736778
C	-3.5231717049	-0.2034429101	1.6932996199
H	-3.4613982004	-1.1595903893	2.2220672556
H	-4.5280500253	0.1984038868	1.859255037
H	-2.8084718418	0.4891390358	2.1507239506
H	-3.3382625522	0.9935331899	-1.5564963111
H	-2.8622503999	1.7766513283	-0.0433819765
H	-4.5496727925	1.3227731776	-0.3187212711
H	-4.1706994707	-2.3582398588	0.0681548105
H	-4.2051375981	-1.4728054142	-1.462426999
H	-5.3299643192	-1.0330999257	-0.1619219146
H	-0.4755993254	1.3716012245	0.369547052
H	-0.9225169418	1.9861320646	-1.2158472154
C	0.9579420802	2.7568170287	-0.4885905535
H	1.7816730293	2.4211374434	0.155591922
C	0.3720156343	4.064296444	0.066919508
H	1.4024781845	2.9508213908	-1.4737113947
H	-0.427479182	4.413717885	-0.6009999786
H	1.1493041487	4.8387943778	0.0423308666
C	-0.1734423994	3.9470494215	1.4952021611
H	0.5959868568	3.5687213782	2.1786258177
H	-1.0271199385	3.2637333514	1.5500117085
H	-0.5068560158	4.9190237226	1.8731541068
C	3.3862361688	-2.0664319497	-0.3882266806
H	2.9946408439	-0.6416073273	-1.9484626474

H	1.8537120904	-1.9648239752	-1.9154094524
H	2.8351771634	-2.7304379825	0.2884787931
C	4.3448097249	-1.1926202639	0.431438476
H	3.9805185427	-2.7227373593	-1.038049852
C	5.343122496	-2.0183030713	1.2480965893
H	3.7741763836	-0.5439749178	1.1076774532
H	4.8872847077	-0.5202804129	-0.247323329
H	4.8240921562	-2.6763472791	1.9545692841
H	6.019842213	-1.37865952	1.8239105751
H	5.9556714247	-2.6528850309	0.5973458135
H	5.9556714247	-2.6528850309	0.5973458135

TS endo 0446

E(RB3LYP) = -706.412356260 A.U.

First frequency = -524.2959 cm^{-1}

H	-1.3369952673	-0.1535069891	-2.1215308912
C	-1.165937631	-0.8483476092	-1.3074746617
H	-0.464918349	-1.6369717331	-1.5521286142
C	-2.1361978463	-1.0560840462	-0.3299010514
C	-1.7923690751	-1.8827460976	0.7623552736
C	-0.5681228711	-2.5254568128	0.85844143
H	-0.3121659086	-3.0527171294	1.7736079179
H	-0.0928060421	-2.9241239188	-0.0299573153
C	1.0325557246	-0.9552044468	0.675659631
H	0.9465181083	-0.7893617873	1.747616943
C	2.1819556484	-1.8513639598	0.2616263915
C	0.5259960143	0.0518925047	-0.152068989
H	1.002372584	0.2064450125	-1.1163211157
C	-0.1530791471	1.2457395901	0.4797283384
C	-3.4945633434	-0.3220451308	-0.3273212726
H	-2.4298516174	-1.8680049842	1.6431491429
C	-3.6386491571	0.6490871542	-1.5130075698
C	-3.7332585317	0.4820904146	0.9711655052
C	-4.5963635896	-1.4030579198	-0.4498653002
H	-4.4682640387	-1.9861518081	-1.3675816753
H	-5.5900678672	-0.9404697307	-0.4723483441
H	-4.5656006435	-2.0989354955	0.3941195303

H	-3.6552523388	-0.1416385322	1.8656488261
H	-4.7388627548	0.9175218655	0.9625735032
H	-3.0151266073	1.3006760997	1.0669825263
H	-2.8847512844	1.4426748745	-1.4790037264
H	-4.6233639626	1.1269133759	-1.4833990005
H	-3.5492788463	0.1327158057	-2.4738670106
H	-0.8918495151	0.8676584346	1.1957078122
H	-0.7165378629	1.8026048439	-0.2768000308
C	0.7923786638	2.2050222013	1.2333108839
H	0.1849434756	3.0134688195	1.6643319826
C	1.9181400403	2.8201936976	0.3887322495
H	1.2400169513	1.6687721287	2.0797405064
H	2.6131413968	2.0298974153	0.0835114634
H	2.497401485	3.5028414956	1.0235463273
C	1.4305928996	3.5750004706	-0.8521818778
H	0.7058818431	4.3525139146	-0.5831629272
H	0.9423007441	2.9033706691	-1.5662882847
H	2.2625269632	4.0596305208	-1.3733920065
C	3.5744452986	-1.1871177044	0.3794906925
H	2.0354714344	-2.1886322473	-0.7749019782
H	2.1712843131	-2.7566721161	0.8795955031
H	3.6011913418	-0.5677155234	1.2865455425
C	3.9739190739	-0.3400342583	-0.834373819
H	4.3347905441	-1.9669908307	0.522475432
C	5.2911329736	0.4120743663	-0.6284672865
H	3.1790181699	0.378209032	-1.0613541222
H	4.0509388132	-0.9941232811	-1.7136400821
H	6.1111268782	-0.2788227551	-0.4010378832
H	5.2115369343	1.1162989204	0.2077673931
H	5.5723606115	0.9832027869	-1.5192504989
H	5.5723606115	0.9832027869	-1.5192504989

TS endo 0452

E(RB3LYP) = -706.410346076 A.U.

First frequency = -514.1731 cm^{-1}

H	-0.8335972389	-0.2110246701	-2.1189320856
C	-0.6335098818	-0.7492203074	-1.1972342536

H	0.1978494306	-1.4360908616	-1.2644685642
C	-1.6456290337	-0.9459365938	-0.2632633456
C	-1.2969236867	-1.544022056	0.9689008774
C	-0.0160315706	-1.9928576183	1.2478693871
H	0.2191221304	-2.3413772539	2.2498132881
H	0.5885687725	-2.4412016599	0.4685491524
C	1.3694389	-0.2495650118	1.0151142186
H	1.0784237571	0.0598332582	2.0166520912
C	2.6975184187	-0.9873610835	0.9617124593
C	0.8848287581	0.5377895778	-0.0292220001
H	1.4606812591	0.5934552128	-0.9488428181
C	0.0197455872	1.7341239204	0.2857005144
C	-3.0799942125	-0.442516969	-0.5435485687
H	-1.9957677621	-1.4816667304	1.796502656
C	-3.6803422049	-1.3643801177	-1.6338807294
C	-3.1087798512	1.0128974729	-1.058513924
C	-3.9884737051	-0.5146334132	0.69841236
H	-4.0864043275	-1.5380182896	1.073762486
H	-4.9928100806	-0.161725084	0.4422624215
H	-3.6123416191	0.1153024332	1.5114482208
H	-4.1312632568	1.2868554661	-1.3412831396
H	-2.4782344642	1.1550722666	-1.9403408938
H	-2.7751240765	1.7116608178	-0.2873443549
H	-3.6788620372	-2.4083939827	-1.3039047487
H	-3.0994844375	-1.3060934326	-2.5595018587
H	-4.7142389314	-1.0774547051	-1.8598748365
H	-0.7681333915	1.4224533219	0.9860404433
H	-0.4855429319	2.0744978633	-0.6212965041
C	0.803932786	2.905082811	0.9075589983
H	1.3478995673	2.5403634593	1.7879332789
C	-0.0806517807	4.0938747138	1.3152176186
H	1.5693945879	3.246251652	0.1960500419
H	0.5410260535	4.8355162681	1.8330992007
H	-0.8232263058	3.7520488363	2.0496472185
C	-0.7997405827	4.7742048214	0.1442026053
H	-0.0836738325	5.0982407882	-0.6203099451
H	-1.3525704889	5.6580564761	0.478957378
H	-1.5168257985	4.1026910244	-0.3388710047

C	3.1294482787	-1.5164859627	-0.4117305208
H	2.681701018	-1.8247437683	1.6720798005
H	3.480844837	-0.3077633748	1.3323294009
H	2.352072804	-2.1735487401	-0.8244998557
C	4.4544474119	-2.2858254211	-0.3603194639
H	3.2290281714	-0.6838156838	-1.1197093451
C	4.8959676788	-2.8054342983	-1.7312934386
H	4.3570800006	-3.1271193749	0.3391724939
H	5.2341478197	-1.6335410131	0.0560296706
H	4.1466743694	-3.483785603	-2.1552833513
H	5.8428324249	-3.3514250634	-1.6691489263
H	5.0318973615	-1.9807162059	-2.4402638986
H	5.0318973615	-1.9807162059	-2.4402638986

TS endo 0462

E(RB3LYP) = -706.409279645 A.U.

First frequency = -525.3143 cm⁻¹

H	-1.8408646903	0.4220459225	-1.9775749088
C	-1.4450007054	-0.4293134424	-1.4359677321
H	-0.7843803106	-1.0495975561	-2.0299437969
C	-2.1468138782	-0.9834105209	-0.3671071691
C	-1.5131171233	-2.0125631074	0.363066626
C	-0.2706086238	-2.5200512017	0.0165176638
H	0.2216752582	-3.2268069451	0.6793006568
H	-0.0015976057	-2.6305601014	-1.0271451459
C	1.1575549914	-0.7790766751	-0.0867647791
H	1.3201704237	-0.91577879	0.9774885044
C	2.1804298384	-1.3876482048	-1.0253468629
C	0.4181137684	0.3422348752	-0.4764386099
H	0.651566842	0.7804994135	-1.4431241301
C	-0.1585633053	1.2535895062	0.5838658593
C	-3.5026322848	-0.4311763173	0.123583163
H	-1.9246259166	-2.289424098	1.3308264838
C	-4.5423758407	-1.5676665149	-0.0342593814
C	-3.9796630169	0.7750650066	-0.7052713274
C	-3.4645859203	0.0018003237	1.6071645519
H	-3.1421149306	-0.8081534471	2.2669334555

H	-4.4640786125	0.3112673274	1.9330831473
H	-2.7874448279	0.84709586	1.7551485596
H	-4.9543668709	1.1142094396	-0.3394247227
H	-4.0925305654	0.5206647048	-1.7637821282
H	-3.2859488753	1.6188756999	-0.6279059698
H	-4.2732250476	-2.4394093175	0.5699150295
H	-4.6074378307	-1.8925422735	-1.0777389208
H	-5.5356119019	-1.2287249775	0.2828413017
H	-0.6489570812	0.6053195578	1.3195585348
H	-0.9481215373	1.8845896561	0.1572626747
C	0.8458014881	2.1528353884	1.3406563268
H	0.3685046396	2.4609769183	2.2805742831
C	1.2956043686	3.4286397078	0.6097672998
H	1.7233890863	1.5587987335	1.6238208072
H	1.8241496027	4.0665568179	1.3304421092
H	0.4045332911	3.995001362	0.3047304948
C	2.2037731402	3.2169560753	-0.6064307461
H	1.6938595217	2.6802050169	-1.4108040149
H	3.0930917916	2.6372504789	-0.3365355148
H	2.5425728426	4.1757448854	-1.013481559
C	3.5078948797	-0.6105867674	-1.189426877
H	1.7170193443	-1.4644682275	-2.0196221999
H	2.4126833388	-2.416602256	-0.7212724977
H	3.9714270797	-0.9433793565	-2.1276867953
C	4.5451264723	-0.7974842901	-0.0696632659
H	3.2875007329	0.4562546673	-1.317718746
C	4.1970191337	-0.1599320371	1.2797051551
H	5.4980577436	-0.3763864021	-0.4162902429
H	4.7256909821	-1.8724434216	0.0703605113
H	5.0253970623	-0.2680928467	1.988065257
H	3.3139296071	-0.6165240982	1.7340734069
H	3.9926837975	0.910247493	1.1674131938
H	3.9926837975	0.910247493	1.1674131938

TS endo 0469

E(RB3LYP) = -706.408886820 A.U.

First frequency = -549.1642 cm^{-1}

H	-1.7741515356	-1.591943131	-1.8688643693
C	-1.3909870048	-1.5942914503	-0.8546553577
H	-0.74728044	-2.4396472376	-0.6413930123
C	-2.1112645431	-0.9928256474	0.1779441825
C	-1.5008310893	-0.9397561351	1.4487651115
C	-0.2627303725	-1.5069317772	1.7054961595
H	0.2197494527	-1.3283915734	2.6628715621
H	0.0088270091	-2.4475731892	1.2416540844
C	1.1689475885	-0.6665663512	0.1841233868
H	1.3590941054	0.1469600889	0.8732477146
C	2.1814599936	-1.7958334977	0.1958440838
C	0.4643266756	-0.3922971925	-0.9949643974
H	0.7210773528	-1.0156372605	-1.8507452189
C	-0.0230567213	1.0002044575	-1.3833531411
C	-3.4637495131	-0.2821380798	-0.0423736051
H	-1.9217599884	-0.2720883536	2.1972265884
C	-3.4114948035	1.2112869799	0.3503546564
C	-4.5097200193	-0.9954451948	0.8489789821
C	-3.9428481239	-0.3691096012	-1.5027379332
H	-3.2537387102	0.1349163032	-2.1887752452
H	-4.9188833723	0.117132848	-1.6021975913
H	-4.0525985122	-1.4072786059	-1.8316759446
H	-5.4994734515	-0.5423857894	0.7185421683
H	-4.244229587	-0.9273951777	1.9081804898
H	-4.5814213902	-2.0569621929	0.5908601209
H	-4.407593872	1.6597478421	0.2617821836
H	-2.7341693271	1.7659315145	-0.3028447146
H	-3.0758137661	1.35648186	1.3806191433
H	-1.0397585202	0.9300227186	-1.7826618492
H	0.5954734918	1.3466972986	-2.2257020692
C	0.0149952281	2.0762909692	-0.282668213
H	-0.7190036629	2.8567225422	-0.5205879831
C	1.3835182642	2.7510180365	-0.1143221046
H	-0.3144072385	1.6424347958	0.6692411884
H	1.6264003574	3.2901596913	-1.0400713512
H	2.163510685	1.9900624887	-0.0010682652
C	1.4280433533	3.7150809076	1.07351109
H	2.4025190817	4.2068807891	1.1591231419

H	1.236632554	3.1864075873	2.0145983156
H	0.6661235731	4.4971967229	0.9762117155
C	3.518091265	-1.4438216536	-0.4877974536
H	1.7472441127	-2.6670799416	-0.315064866
H	2.3875690874	-2.1144965997	1.2257823051
H	4.1225240919	-2.3573238274	-0.578996517
C	4.3372311216	-0.3822435054	0.255105832
H	3.318205272	-1.1003346242	-1.5117235591
C	5.66228186	-0.05999922	-0.4409895954
H	4.5313214864	-0.7303206426	1.2791442003
H	3.7460010744	0.5361112482	0.353466875
H	6.2331149769	0.6955669511	0.1086456588
H	5.4903435651	0.3228754775	-1.4534902006
H	6.289951822	-0.9542571879	-0.5294593921
H	6.289951822	-0.9542571879	-0.5294593921

TS endo 0474

E(RB3LYP) = -706.410444793 A.U.

First frequency = -498.8421 cm^{-1}

H	-1.9592086554	-0.6789955106	-2.1668876932
C	-1.4079906626	-1.1146071958	-1.3388135621
H	-0.7124583973	-1.8882519026	-1.6385709207
C	-1.9427803108	-1.0997765104	-0.0546379874
C	-1.1332648976	-1.5850278901	0.9990497749
C	0.109053437	-2.1562512219	0.793103223
H	0.7244315059	-2.4145341135	1.6494532935
H	0.3070958512	-2.741122608	-0.0970085178
C	1.3630336327	-0.5964647827	-0.3454918216
H	1.6147412647	-0.191153669	0.629476113
C	2.396432127	-1.4917087167	-1.0011250357
C	0.4770963658	0.1436198529	-1.1235821183
H	0.5761185333	0.0683167716	-2.2053954774
C	-0.0787193644	1.4413659342	-0.5909869081
C	-3.3404251664	-0.4958456663	0.2079100158
H	-1.4114298389	-1.3503868595	2.0213492085
C	-3.6384947319	-0.3186866175	1.7089137713
C	-4.3797646809	-1.4843568475	-0.3768586869

C	-3.5303267894	0.8778379673	-0.4705471727
H	-3.3285187565	0.8433629464	-1.5445933896
H	-2.875013316	1.6313700008	-0.027034825
H	-4.5652280935	1.2148491343	-0.3442366715
H	-4.2770977442	-2.4731236572	0.0820760001
H	-4.2442140606	-1.6016184455	-1.4564561002
H	-5.4006510075	-1.1268859422	-0.1969061341
H	-4.6415298625	0.1005629991	1.8391101224
H	-2.9279485874	0.3661863299	2.183740012
H	-3.6092219625	-1.2714535679	2.2466319312
H	-0.4997737451	1.258382837	0.4075507426
H	-0.9061493566	1.784539491	-1.2202953135
C	0.9737556734	2.5605170506	-0.494020933
H	1.8002796931	2.2281908468	0.1484579038
C	0.3992180583	3.8739977839	0.0481110016
H	1.4137676584	2.7352100246	-1.4859796505
H	-0.0451599816	3.691094129	1.0362406408
H	-0.4259774633	4.2022271063	-0.5986684117
C	1.445336437	4.9873767017	0.1523810783
H	1.8820332733	5.2100920744	-0.8279345954
H	2.265179106	4.6956229486	0.818791687
H	1.0116030735	5.9139120335	0.5427338359
C	3.2638580692	-2.3446460731	-0.0582674633
H	3.0623433358	-0.8600823102	-1.6062821064
H	1.8975022693	-2.1527463376	-1.7249055893
H	2.6581391875	-3.1387023405	0.3921745404
C	3.9687904267	-1.5630745205	1.0633961275
H	4.0247956219	-2.8512348636	-0.6669327725
C	4.825294765	-0.3930261125	0.5673710813
H	4.598658243	-2.2619986591	1.6280488591
H	3.2242927896	-1.1906985634	1.7784986416
H	4.2113422156	0.382034631	0.0969061375
H	5.5609895585	-0.7282071963	-0.173151304
H	5.3717913807	0.0750190937	1.3924511761
H	5.3717913807	0.0750190937	1.3924511761

TS endo 0480

E(RB3LYP) = -706.409805104 A.U.

First frequency = $-529.9974 \text{ cm}^{-1}$

H	-1.9700866727	-0.4157568282	-2.251342973
C	-1.4245516728	-0.9041862747	-1.4516172388
H	-0.7111957033	-1.6397932526	-1.8072533963
C	-2.0025106283	-1.0558828099	-0.1901788713
C	-1.197270489	-1.6103377922	0.8273990722
C	0.0918704112	-2.0623851063	0.610714637
H	0.6937036027	-2.3684979102	1.4610327255
H	0.3651853703	-2.5336584403	-0.3253369501
C	1.2244912362	-0.2995356118	-0.3832956139
H	1.445122147	0.0188008629	0.6279950399
C	2.3019207874	-1.0657014934	-1.1307079669
C	0.2704965046	0.4257514318	-1.1053698302
H	0.4129211991	0.4662534037	-2.1861811704
C	-0.3814581878	1.6539027224	-0.5078985877
C	-3.4030451743	-0.516012562	0.1680023649
H	-1.5338686295	-1.5195368595	1.8577250994
C	-4.2629298776	-1.7224422525	0.6182956699
C	-4.1032464509	0.1464359142	-1.0322783094
C	-3.3542089743	0.5153310196	1.3190397184
H	-2.8872263571	0.1062576802	2.2190915645
H	-4.3697449708	0.8267904046	1.5889195421
H	-2.7949968126	1.4075884725	1.0266370302
H	-3.5557920345	1.0245671664	-1.3903401565
H	-5.1041454729	0.4802516135	-0.7395512591
H	-4.2163283082	-0.5497710288	-1.8693352488
H	-4.3323126548	-2.4693383946	-0.1791748835
H	-5.2782757469	-1.3976244549	0.8742049973
H	-3.8337452283	-2.2125946854	1.4972818227
H	-0.5316007597	1.4896681936	0.5649366433
H	-1.3794628817	1.7954221957	-0.9363133976
C	0.4154128525	2.9560350942	-0.7435052891
H	0.5269193051	3.1012691941	-1.8266771875
C	1.8019063659	3.0283677102	-0.0874084018
H	-0.1908872751	3.7994925731	-0.3841159118
H	2.2932413669	3.9539061923	-0.4136636592
H	2.4229122051	2.2058085944	-0.4619249665

C	1.7677930409	2.996656391	1.444130728
H	1.3544764625	2.0568649595	1.8234705817
H	1.1486752227	3.8107593475	1.8387252871
H	2.7721522945	3.1049875716	1.8660970894
C	3.3082505695	-1.8752939472	-0.2901964609
H	2.8690923165	-0.3627120439	-1.76052841
H	1.806822073	-1.7417126476	-1.8444211011
H	2.7851154212	-2.3918795484	0.5227158458
C	4.4866434122	-1.076834911	0.29377175
H	3.7271065381	-2.6635616741	-0.9281334995
C	4.1167382502	-0.0329339027	1.3529635007
H	5.0247448543	-0.5840678289	-0.5278860324
H	5.195625949	-1.79047647	0.733347194
H	5.014247193	0.4059112209	1.8015637279
H	3.5260322916	-0.4813598851	2.1604118391
H	3.5301593934	0.7851430878	0.9291655741
H	3.5301593934	0.7851430878	0.9291655741

TS endo 0483

E(RB3LYP) = -706.411647382 A.U.

First frequency = -529.6056 cm^{-1}

H	-1.1940649174	0.1043695029	-1.9637839675
C	-1.0111216725	-0.657147791	-1.215347561
H	-0.2966173661	-1.4077393172	-1.5261903852
C	-1.9617773996	-0.9496440557	-0.2429878481
C	-1.607327328	-1.8760315465	0.7620823349
C	-0.3913151004	-2.548005324	0.7572022256
H	-0.1326160664	-3.1815923384	1.6018450676
H	0.0221900528	-2.887197187	-0.186301053
C	1.2252820859	-1.0910326482	0.7476431456
H	1.1834778863	-1.049075562	1.8354069581
C	2.3534553546	-1.9401179717	0.1930579301
C	0.7837254356	0.0550896345	0.0748619404
H	1.2457551112	0.3059149414	-0.8743560701
C	0.168235757	1.1769949175	0.8787848397
C	-3.3256432755	-0.2297224012	-0.151192036
H	-2.2233239913	-1.9354228485	1.6562100072

C	-3.4929466486	0.5401534463	1.1781512362
C	-4.425861062	-1.3159994495	-0.2382841109
C	-3.5492299878	0.7619114621	-1.3073789274
H	-3.4816051096	0.266902673	-2.2812273209
H	-2.825179473	1.5814547536	-1.287177482
H	-4.5477432033	1.2042825746	-1.2270498884
H	-5.4209446933	-0.8575299661	-0.2020768066
H	-4.3532437206	-2.0293934994	0.5878607163
H	-4.341895581	-1.8793515692	-1.1732535313
H	-2.7801422516	1.3660307529	1.2487237748
H	-3.3485146852	-0.105370514	2.0488080404
H	-4.5017221675	0.9633312151	1.2445988882
H	0.8788655588	1.4886626782	1.660518422
H	-0.6827146613	0.7486040302	1.42499125
C	-0.2765071028	2.4246049654	0.0953705859
H	-0.688007459	2.1163360957	-0.8724936431
C	0.8139923325	3.4847299124	-0.1343151596
H	-1.1008748091	2.9058625972	0.6363027085
H	1.1995758907	3.8169877604	0.8394314555
H	0.3470884386	4.3665956526	-0.591952108
C	1.9842951616	3.0293832011	-1.0117490741
H	2.6797542434	3.8537756174	-1.2014791707
H	1.6305888962	2.6615537472	-1.9821918917
H	2.5514691915	2.2233491667	-0.5404525277
C	3.7473440763	-1.5217264238	0.7098814498
H	2.3309710765	-1.9026283207	-0.9040380188
H	2.209649754	-2.9940443154	0.4619749552
H	3.7493901502	-1.6169759089	1.8041439433
C	4.2035376704	-0.1049424113	0.3339879083
H	4.4864344908	-2.245497845	0.338813072
C	4.3957585276	0.1093207842	-1.1708345403
H	5.1503426512	0.1040281786	0.8479778334
H	3.4791038801	0.6210730061	0.7223587105
H	5.1134735134	-0.6108718517	-1.5806695707
H	4.7715601249	1.1152074281	-1.3835606285
H	3.4578350058	-0.0103800152	-1.722035724
H	3.4578350058	-0.0103800152	-1.722035724

TS endo 0484

E(RB3LYP) = -706.410600121 A.U.

First frequency = -538.3799 cm⁻¹

H	-1.5003676751	0.5608395509	-1.940530035
C	-1.0363109885	-0.2158335326	-1.3439347795
H	-0.2852417071	-0.7821376011	-1.8802381344
C	-1.7038564553	-0.7804361328	-0.2620157286
C	-0.9927772609	-1.7051937889	0.5353548578
C	0.2811073437	-2.1522241309	0.2153763837
H	0.803089751	-2.7957778689	0.9177329001
H	0.5422253431	-2.3248053505	-0.8226429165
C	1.6201148613	-0.3823702322	-0.0018225082
H	1.8650194128	-0.4916251991	1.0509142385
C	2.6467444507	-0.8980973083	-0.9954309913
C	0.8167362054	0.7071521426	-0.3422942685
H	0.9889863314	1.1826166541	-1.3048922832
C	0.2282016501	1.5530768709	0.7600629792
C	-3.1259432804	-0.3572597088	0.1692510867
H	-1.3892113252	-1.9533782254	1.5174112195
C	-3.782135899	0.6106887649	-0.8326040109
C	-3.1390984586	0.3095827604	1.5632353112
C	-3.9958162509	-1.6375765316	0.2216428335
H	-3.6182077119	-2.3535316392	0.957233246
H	-4.0104517072	-2.1372829392	-0.7523318533
H	-5.0276487709	-1.387854222	0.4946463023
H	-2.67550794	-0.3245678309	2.3242418303
H	-4.1702699758	0.5056329799	1.878870449
H	-2.6075260302	1.2645083759	1.5494595629
H	-3.8243322032	0.1798985901	-1.8379383244
H	-3.2504999194	1.5649667549	-0.8915225935
H	-4.8081200647	0.8290125633	-0.5181459308
H	1.0419359048	1.89893802	1.4163815164
H	-0.3928715425	0.9002284969	1.3880734418
C	-0.5761400763	2.7725565941	0.2975424432
H	-1.3578355022	2.4475974016	-0.3984176167
C	0.2689693798	3.8652683556	-0.3702675785
H	-1.0957028008	3.2099990881	1.1607722886

H	0.7975862727	3.4492506248	-1.2373888969
H	1.0487863401	4.1949884312	0.329749
C	-0.5676227493	5.0676197905	-0.8167312142
H	0.0512935336	5.8386132093	-1.287108127
H	-1.0836304784	5.5264450965	0.0345621709
H	-1.3333608868	4.7661074359	-1.5408487771
C	3.480961475	-2.1087410133	-0.548501297
H	3.3404461734	-0.0786560643	-1.2375448576
H	2.1402510623	-1.1357398601	-1.9427727654
H	2.8281890794	-2.9653729517	-0.3423812774
C	4.3674166344	-1.8449429058	0.6756466998
H	4.1229903842	-2.4142029644	-1.3856208142
C	5.2356080171	-3.0512301902	1.0453233905
H	3.7444893413	-1.5720137617	1.5365061509
H	5.0076347109	-0.9747248742	0.4758578445
H	4.6160093947	-3.9253803842	1.2765581105
H	5.860913967	-2.8451045762	1.9200451491
H	5.8988744547	-3.3282804505	0.2178718088
H	5.8988744547	-3.3282804505	0.2178718088

TS endo 0491

E(RB3LYP) = -706.409005083 A.U.

First frequency = -540.9873 cm^{-1}

H	-1.2009553623	-1.4174443624	-2.0705669414
C	-1.0194576862	-1.5246954388	-1.0071807966
H	-0.359060604	-2.3479861082	-0.7632528572
C	-1.9614156911	-1.0912320277	-0.0754680694
C	-1.6048967853	-1.1607550054	1.2880214729
C	-0.3872709058	-1.66694939	1.7131123151
H	-0.1089651447	-1.5831696681	2.7603959452
H	0.0579569192	-2.5138489777	1.2040042911
C	1.1955621547	-0.5091636372	0.6402844493
H	1.1199549507	0.2585007695	1.4027702035
C	2.3517260874	-1.4700783217	0.83577217
C	0.7375972398	-0.2004537436	-0.6478686295
H	1.225086335	-0.7351418349	-1.4603139332
C	0.2244436181	1.1808886073	-1.0508503926

C	-3.2911784394	-0.4157087674	-0.4726452546
H	-2.2127544667	-0.6209452178	2.010504473
C	-4.4399978493	-1.2646232727	0.1242627996
C	-3.4872764995	-0.3549592391	-1.9982946792
C	-3.3977387972	1.0243374826	0.0784490655
H	-4.379235026	1.4490100479	-0.1615000729
H	-2.6348200861	1.6720568985	-0.359790548
H	-3.2809891068	1.0593952147	1.1649750104
H	-4.4583559263	0.0949742252	-2.2296304877
H	-3.4658634203	-1.352437395	-2.4484943192
H	-2.7191675879	0.2550691049	-2.4853802094
H	-4.4026202436	-2.2908970113	-0.2551463119
H	-5.4132451834	-0.8354398742	-0.1410923473
H	-4.3782634312	-1.3104877031	1.215599547
H	-0.725044418	1.082477058	-1.585322054
H	0.9296480008	1.5923560237	-1.7891542148
C	0.0587376207	2.213456221	0.0777534397
H	-0.6287801144	2.999415037	-0.2615152442
C	1.3693806458	2.8840379933	0.5138879551
H	-0.4329681315	1.7455254632	0.939876605
H	1.7826897057	3.436102727	-0.3412239181
H	2.1156457086	2.1218558636	0.7657366243
C	1.1827431378	3.8328290502	1.7006342693
H	2.122145508	4.3212936714	1.9793996023
H	0.8134762341	3.2926199845	2.5801915029
H	0.4538111309	4.6179317492	1.4683671075
C	3.7319705764	-0.776529657	0.7728650361
H	2.2992893261	-2.2685421503	0.0836561194
H	2.2768635242	-1.9665502356	1.8108786053
H	3.758590202	0.0020605262	1.5473652452
C	4.1090258279	-0.1485336968	-0.5773408983
H	4.5020309195	-1.5099337285	1.0507352729
C	4.2771710199	-1.1646100708	-1.7120218341
H	5.0490948443	0.4035144277	-0.4512279106
H	3.3541669211	0.595507567	-0.8576880604
H	3.3430212282	-1.6928235544	-1.9284066904
H	5.0287919571	-1.9202743228	-1.4550424919
H	4.5983164289	-0.6754546858	-2.6374093705

H 4.5983164289 -0.6754546858 -2.6374093705

TS endo 0492

E(RB3LYP) = -706.409130208 A.U.

First frequency = -510.7738 cm⁻¹

H -1.6545584333 -0.438943108 -2.2673459412
C -1.1693031143 -0.844772538 -1.3842554047
H -0.2813469266 -1.4240797492 -1.6057453998
C -1.9119305517 -1.1019880322 -0.2340003506
C -1.2104316066 -1.5296920252 0.9155307705
C 0.1470823368 -1.794585643 0.9160695731
H 0.6417357338 -2.0136940849 1.8572056296
H 0.6290875558 -2.2205113218 0.0441860961
C 1.1878886419 0.1099618583 0.1465521126
H 1.1839102292 0.4375227823 1.1818012716
C 2.4838880078 -0.4862538444 -0.3689384024
C 0.3063803383 0.7363641688 -0.7334135844
H 0.6141699217 0.7966555471 -1.7771617226
C -0.6010910343 1.8486996972 -0.2635956302
C -3.4364133297 -0.8525643167 -0.2077107675
H -1.7100615058 -1.4854946456 1.8778326032
C -4.0923867961 -1.9497716713 -1.082587476
C -3.8223448933 0.5286534895 -0.7779828572
C -4.0296211217 -0.9528644499 1.2105051686
H -3.8674850374 -1.9410491012 1.6520144442
H -5.1107686573 -0.7843478912 1.1710400309
H -3.6006975685 -0.2016732696 1.8820932139
H -3.4345328446 0.684421273 -1.7884929831
H -3.4486054373 1.335427259 -0.1423965762
H -4.9131084494 0.6186367198 -0.8304500835
H -5.1840751859 -1.8467708508 -1.0814878089
H -3.8420028265 -2.9474356917 -0.7074626944
H -3.7446040438 -1.8854063644 -2.1182058025
H -1.0296033091 1.5708218658 0.7090547912
H -1.4410231953 1.9528587752 -0.9550939889
C 0.0876360513 3.2266863679 -0.1498375718
H 0.5106638457 3.4975644172 -1.1278449248

C	1.1816799194	3.3409866281	0.9172919324
H	-0.6884824394	3.9763609265	0.0601877899
H	2.0002239285	2.6519490112	0.6808520799
H	0.7777746443	3.0135639463	1.8855471803
C	1.7329035109	4.7644968733	1.0436942792
H	2.1624818352	5.1052203837	0.0944492666
H	2.5174742276	4.8263039262	1.8050426458
H	0.9431368035	5.4727749025	1.319582499
C	3.3791154328	-1.1087344533	0.7100212277
H	3.0599794983	0.3026503968	-0.8769773435
H	2.2587653204	-1.2257367505	-1.1511707147
H	3.5213299753	-0.370059729	1.5104597676
C	4.7537241897	-1.5617893951	0.19575692
H	2.8709208021	-1.9642613785	1.1706214152
C	4.6909580459	-2.7066195486	-0.8222005982
H	5.3635366082	-1.8776156976	1.0516409499
H	5.2751339809	-0.7034029713	-0.2498532664
H	4.1568811845	-3.569800432	-0.4076844173
H	5.6943416149	-3.040193738	-1.1060368623
H	4.1734367204	-2.4076972104	-1.7393715056
H	4.1734367204	-2.4076972104	-1.7393715056

TS endo 0499

E(RB3LYP) = -706.410455840 A.U.

First frequency = -516.1538 cm^{-1}

H	-1.234913645	-0.7115761015	-2.1826570952
C	-0.9410715132	-1.0358695147	-1.1892773906
H	-0.2727123985	-1.8873516215	-1.1923657037
C	-1.7751907806	-0.8060630916	-0.0972299869
C	-1.2919020754	-1.165482321	1.1817108107
C	-0.067881392	-1.7810620015	1.371111415
H	0.3126829551	-1.9183796224	2.3794439356
H	0.3022586972	-2.5022301811	0.6525407727
C	1.4961078309	-0.4435707987	0.398926261
H	1.5252560653	0.1507799473	1.3067415416
C	2.5889192733	-1.4840638323	0.2697513821
C	0.9487310975	0.1328166144	-0.7481756813

H	1.3237105156	-0.2505459967	-1.6969290918
C	0.5026443495	1.5832917096	-0.8164191612
C	-3.1470603241	-0.1204544236	-0.2806138006
H	-1.7937390603	-0.7685531347	2.0582637941
C	-4.1123410192	-1.1917194323	-0.8470703835
C	-3.0922519237	1.0619880933	-1.2703918293
C	-3.7355020117	0.4050923615	1.0434346304
H	-4.7032216793	0.8808844537	0.8539406083
H	-3.0836461941	1.1515573027	1.5097370028
H	-3.9046168447	-0.399990882	1.7647792014
H	-2.4624622829	1.8682552125	-0.8892009151
H	-4.0990836174	1.4661642677	-1.421997601
H	-2.7119993185	0.76817638	-2.2522035628
H	-5.1184858772	-0.777068852	-0.9820729615
H	-4.1827968153	-2.0489275838	-0.1696679506
H	-3.759869178	-1.5590148171	-1.8159955458
H	-0.2530764066	1.6999656075	-1.6011507361
H	1.3665147918	2.1817251263	-1.1493628991
C	-0.0298571999	2.1865897232	0.4875838221
H	-0.8547209925	1.5709300865	0.8613590868
C	-0.4951367412	3.638137703	0.3286834865
H	0.748190591	2.1518657009	1.2608745544
H	-1.2429885621	3.7000944248	-0.4734390552
H	0.3509196331	4.2557441268	-0.0025075405
C	-1.0843482183	4.2139399553	1.6192445097
H	-1.9572066056	3.6346965805	1.9426170657
H	-1.4029612116	5.2534482292	1.4904413265
H	-0.3517841767	4.1868789945	2.4340277875
C	3.9657271524	-0.8513057899	-0.0085391195
H	2.3329380094	-2.1760559336	-0.543903912
H	2.6588628953	-2.0914127079	1.1816979072
H	3.9156716516	-0.291225059	-0.9522422595
C	5.1230004165	-1.8601626347	-0.0684120565
H	4.1737492566	-0.1098191756	0.7742467062
C	5.0234000772	-2.8567533711	-1.2291610556
H	5.1732192397	-2.4088922848	0.8822186448
H	6.0678104039	-1.307851748	-0.15095764
H	4.9525974719	-2.3327981032	-2.1896661255

H	4.1425777695	-3.5004401116	-1.1385421685
H	5.9024466581	-3.5082368572	-1.2688558876
H	5.9024466581	-3.5082368572	-1.2688558876

TS endo 0502

E(RB3LYP) = -706.410610054 A.U.

First frequency = -524.3668 cm⁻¹

H	-1.493059037	0.2691197429	-2.0008497071
C	-1.192002467	-0.5395088361	-1.3452894449
H	-0.517330336	-1.2466277672	-1.8104880587
C	-1.9896446094	-0.9286714385	-0.2745313108
C	-1.4784935151	-1.9128390932	0.6015835344
C	-0.2771170652	-2.5686786567	0.3746969328
H	0.1078331564	-3.2472609467	1.1314600591
H	0.0043343696	-2.8337051975	-0.6381988551
C	1.3174810205	-1.0512086637	0.2016975547
H	1.4398655995	-1.1150661233	1.2793587323
C	2.3138371627	-1.8325265702	-0.63101409
C	0.7564312337	0.1267918779	-0.2956174079
H	1.0760467088	0.4592060084	-1.2797574426
C	0.2783488574	1.1754486759	0.6770217898
C	-3.3377830962	-0.2536793982	0.0643837673
H	-1.9542067559	-2.0380476886	1.5717578464
C	-3.2824863149	0.5123428611	1.405343581
C	-4.4066219704	-1.3692788186	0.1713151888
C	-3.7983832273	0.7244047314	-1.0324549953
H	-3.1212278856	1.5771073142	-1.1370857235
H	-4.7864509037	1.1238935487	-0.7808271934
H	-3.8743704008	0.228135595	-2.0050888918
H	-4.472132571	-1.9352303907	-0.763507638
H	-5.3914539031	-0.9353173585	0.3792147275
H	-4.1769680749	-2.0766193728	0.9731485909
H	-2.6018009913	1.3656453562	1.3459578547
H	-2.9498764161	-0.1285225448	2.2269525548
H	-4.2763742921	0.89512938	1.6643818228
H	1.1128588484	1.4472768216	1.3399454055
H	-0.4681010159	0.7110235397	1.3350895859

C	-0.2981498595	2.4540955379	0.0565935586
H	-1.1978245075	2.2008945639	-0.5133859421
C	0.6640432911	3.2288939809	-0.8603006795
H	-0.6224937657	3.1185857682	0.8689341218
H	0.1440678579	4.1214721985	-1.2307925999
H	0.8925354131	2.628508621	-1.7502174541
C	1.9730899013	3.6488435978	-0.1834695067
H	2.5823773024	4.2680401721	-0.8498544223
H	2.5744998665	2.7796660396	0.100748579
H	1.7785375773	4.2284353671	0.7265919991
C	3.6950978968	-1.1678348801	-0.8193649093
H	1.884558746	-1.9954590958	-1.6305535213
H	2.4620082141	-2.8300380566	-0.1975751059
H	4.2589824842	-1.7877752793	-1.5289050585
C	4.5400666608	-0.9930961988	0.4567553876
H	3.5629612994	-0.1909507853	-1.3036270363
C	4.2019619116	0.2434581389	1.2991241577
H	5.5963995149	-0.9289948844	0.1660926462
H	4.4543668458	-1.8984373093	1.0737332971
H	4.8779989119	0.3323324533	2.1563407707
H	3.1793113032	0.2155622236	1.6816972994
H	4.3023796235	1.1567022199	0.7012544485
H	4.3023796235	1.1567022199	0.7012544485

TS endo 0508

E(RB3LYP) = -706.409514078 A.U.

First frequency = -538.9501 cm^{-1}

H	-1.6881887854	-0.7117521902	-2.217216846
C	-1.2913168468	-1.1533790053	-1.3102384196
H	-0.7038765779	-2.0463733473	-1.4875860959
C	-1.9467382885	-0.9870173514	-0.0912268745
C	-1.3140597417	-1.5003271844	1.0623558685
C	-0.1165496285	-2.1935628854	1.0127073449
H	0.3906742999	-2.4540126567	1.9378671801
H	0.0907664601	-2.8653735512	0.1885186556
C	1.3533995929	-0.8701309404	-0.0822890403
H	1.5806820345	-0.3923712286	0.8632519207

C	2.3252755329	-1.9475716621	-0.516886873
C	0.6622840428	-0.1280207487	-1.0458582115
H	0.8633917456	-0.3967319272	-2.082299819
C	0.3081340829	1.3411590008	-0.8569367392
C	-3.2526444478	-0.1778314901	0.0568698519
H	-1.6761374995	-1.1782827374	2.036159351
C	-3.7434488823	0.3974099772	-1.283982604
C	-3.1066500691	0.9979341814	1.0477814757
C	-4.3352038436	-1.1478061954	0.5904382265
H	-4.47446273	-1.9902032992	-0.0947852647
H	-5.2957542668	-0.6306557126	0.6992672698
H	-4.0579112094	-1.5552285674	1.5673040847
H	-4.0729707052	1.4951628313	1.1893634751
H	-2.3999433981	1.7402351625	0.6710720298
H	-2.7590563743	0.6711201019	2.0314903193
H	-3.9267060599	-0.3908201405	-2.0208690091
H	-3.0233845374	1.103682728	-1.7109808607
H	-4.6840559452	0.9373236204	-1.1334248545
H	-0.7030031702	1.5422155402	-1.2320080886
H	0.9817706484	1.9200026011	-1.5049539776
C	0.4185728876	1.8770635505	0.5765820425
H	-0.1886736028	1.2515279338	1.2399560608
C	-0.0071281288	3.346280792	0.7220189424
H	1.4557803	1.7790984257	0.9243809002
H	-0.026107124	3.6022306669	1.7889128377
H	-1.0378630587	3.468602463	0.3627207145
C	0.9037579108	4.3367412023	-0.0133434334
H	0.8817691781	4.1832828022	-1.0969356798
H	1.9443578711	4.2289589354	0.3146245808
H	0.5991887806	5.3709493933	0.177297568
C	3.6516477671	-1.3803163232	-1.0685202358
H	1.8631204705	-2.5647676992	-1.3003048058
H	2.5384432709	-2.6250786484	0.3179634884
H	4.3109750555	-2.2198441159	-1.3303522662
C	4.3939740655	-0.4341888128	-0.1117641167
H	3.441698622	-0.8436046319	-2.0024867286
C	4.7545493392	-1.0668233155	1.2365100621
H	3.7811020967	0.4603131354	0.0573910105

H	5.3101104109	-0.0864508156	-0.6055822484
H	5.3464133408	-0.380572837	1.8508239644
H	5.3410363226	-1.9828597328	1.0988984574
H	3.8599034084	-1.3319193951	1.8098491513
H	3.8599034084	-1.3319193951	1.8098491513

TS endo 0515

E(RB3LYP) = -706.409644927 A.U.

First frequency = -528.0273 cm⁻¹

H	-0.8979058005	-0.3121096617	-1.9372866971
C	-0.781658312	-0.8851821524	-1.0247580132
H	0.0314256124	-1.5979407879	-1.0599445918
C	-1.8620343003	-1.1093819652	-0.1760562453
C	-1.6009900947	-1.7556919995	1.052452025
C	-0.3347782384	-2.1806077751	1.4196983613
H	-0.1703018376	-2.5630386761	2.423565196
H	0.3474349522	-2.5777038664	0.6770287942
C	1.0166228332	-0.3927796632	1.3301121711
H	0.6241030434	-0.0732842782	2.2934795432
C	2.3588830533	-1.1055660109	1.4268286291
C	0.6077496562	0.3643670386	0.2277548728
H	1.2637530475	0.4083836604	-0.6353188061
C	-0.2658909554	1.5777502478	0.4552630866
C	-3.2791830087	-0.5659668313	-0.4581818915
H	-2.3739177453	-1.7448490468	1.8171803885
C	-3.7989195591	0.3458426708	0.6766799095
C	-4.2212171871	-1.7883319541	-0.5836499983
C	-3.3499491721	0.2327101302	-1.7721614243
H	-2.7074084324	1.1188921446	-1.7414796189
H	-4.3759942883	0.5742709122	-1.9438658058
H	-3.0540701944	-0.3753737108	-2.6327435529
H	-4.2407616341	-2.3725305784	0.3414097988
H	-3.8916890895	-2.4515757648	-1.3899396994
H	-5.2457192565	-1.4646868993	-0.8017231755
H	-4.8323180548	0.6480190111	0.4722327991
H	-3.1954844707	1.2535920153	0.7610928694
H	-3.7908662659	-0.1558882801	1.6479565021

H	-1.0842495303	1.2938633479	1.1262804094
H	-0.7323823675	1.8920583197	-0.4846223394
C	0.4892092424	2.7695358997	1.0817846001
H	-0.2109816935	3.6107136701	1.1839870502
C	1.7263429357	3.2344495949	0.2976818921
H	0.7993587934	2.4962029177	2.0984695746
H	2.482022464	2.4390109621	0.3139867841
H	2.1740701317	4.0880398111	0.8222411271
C	1.4347348304	3.6288261817	-1.1540129031
H	2.330097339	4.0228818691	-1.6456931336
H	0.6578142543	4.4006953494	-1.2054340922
H	1.0867282706	2.7730024042	-1.7422314193
C	3.0159985843	-1.5298151333	0.0974212605
H	2.2514056353	-1.9853102553	2.0725397004
H	3.0558965789	-0.4432571685	1.9634858446
H	3.6253095564	-2.4262963403	0.2686122226
C	3.9157268379	-0.4587555042	-0.5372611547
H	2.2449259178	-1.8318327451	-0.623758241
C	4.4881829434	-0.8912721982	-1.8894334118
H	4.7356652338	-0.2323337439	0.1575883289
H	3.3599162036	0.4780769573	-0.657560725
H	5.1456092	-0.1249974253	-2.3126620146
H	3.6865938249	-1.0799781061	-2.6129562583
H	5.0696701381	-1.815651223	-1.794709608
H	5.0696701381	-1.815651223	-1.794709608

TS endo 0523

E(RB3LYP) = -706.409979878 A.U.

First frequency = -518.0889 cm^{-1}

H	-0.9103939056	-0.502849381	-2.0206664789
C	-0.7017809424	-0.9764409938	-1.0686547423
H	0.1860299338	-1.5937377399	-1.0738266113
C	-1.7213175819	-1.2520750396	-0.163126293
C	-1.3487142666	-1.7597749369	1.1021107968
C	-0.0312862494	-1.9864320457	1.4615515479
H	0.2022364572	-2.2593444418	2.4872092895
H	0.691630381	-2.3330698014	0.7340922726

C	1.025380924	-0.0164925863	1.209004305
H	0.5114332527	0.3381337702	2.1000849431
C	2.4675255996	-0.4279186233	1.4883350827
C	0.5812096277	0.5389894751	0.0043727465
H	1.2701149239	0.5413923706	-0.8360132414
C	-0.4085260386	1.6852292719	0.0433489408
C	-3.2014132118	-0.9051428175	-0.4301331278
H	-2.0984536518	-1.7846103796	1.8893069898
C	-3.7920794543	0.0261997919	0.6531875837
C	-3.992981138	-2.2357567051	-0.4258904948
C	-3.4064993008	-0.2268789291	-1.7965230731
H	-2.8738130993	0.7278212803	-1.8570034519
H	-4.4707362728	-0.0228233348	-1.9535951745
H	-3.0654146623	-0.8624323899	-2.6197106749
H	-5.0553150695	-2.0529260587	-0.6256844276
H	-3.913237865	-2.7437039795	0.5400660054
H	-3.6115803561	-2.916971666	-1.1933800175
H	-4.8584505651	0.1937839756	0.4640432771
H	-3.2953728619	1.0003826234	0.650372125
H	-3.7001407236	-0.3956392081	1.6575089941
H	-1.2228017372	1.4149237617	0.7245170853
H	-0.8611463383	1.8358377961	-0.9444578993
C	0.2146388592	3.0130852452	0.5180038543
H	-0.5779427309	3.7712267206	0.5921181414
C	1.3287726123	3.5413107337	-0.3929981513
H	0.6123191924	2.879769524	1.5334381183
H	0.9422168262	3.6378709417	-1.4173180891
H	2.1393270343	2.802920425	-0.4414933418
C	1.892235991	4.8858817831	0.074884517
H	2.6877815738	5.2431222574	-0.587340603
H	2.3098402387	4.8060847372	1.0852086567
H	1.1104350805	5.6536836614	0.1023373343
C	3.4180824187	-0.6096866787	0.2956135867
H	2.4965380354	-1.339508883	2.100697332
H	2.8917356681	0.3590420047	2.1295330779
H	3.4279360994	0.3044449574	-0.3131430075
C	3.1302258112	-1.8169232288	-0.604027423
H	4.4365295958	-0.7122339933	0.6939758725

C	4.1782545212	-1.9940808621	-1.7065607872
H	2.1419067817	-1.7104948125	-1.0639282406
H	3.0853273272	-2.7246044743	0.0129626788
H	5.1776197916	-2.1401839696	-1.2809678175
H	4.221593836	-1.1094052761	-2.3521996468
H	3.9546294844	-2.8585399058	-2.3399085799
H	3.9546294844	-2.8585399058	-2.3399085799

TS endo 0524

E(RB3LYP) = -706.407987956 A.U.

First frequency = -531.3957 cm⁻¹

H	-0.9892292983	-0.5092943062	-2.0693780756
C	-0.8464731591	-1.0337005225	-1.1316452104
H	-0.1552510242	-1.863388062	-1.1997619427
C	-1.839115113	-1.0385762467	-0.1550311361
C	-1.5271912665	-1.6389583741	1.0844540653
C	-0.2981874448	-2.2239704326	1.3420827039
H	-0.068497202	-2.5633887967	2.348618831
H	0.2272536017	-2.7631586435	0.5622614236
C	1.2686084044	-0.6651680847	0.960808617
H	1.0412344581	-0.2320338925	1.9329835803
C	2.5034837401	-1.5566876404	0.968147118
C	0.8346763256	0.0753293499	-0.1446590701
H	1.3838931339	-0.0160022534	-1.0767393979
C	0.1674552905	1.4112974206	0.0899340389
C	-3.1854105129	-0.3010459666	-0.320211706
H	-2.1926637933	-1.4639445502	1.9264944028
C	-3.3089512111	0.3960099554	-1.6871024678
C	-3.4114107936	0.7659165539	0.775507445
C	-4.3067087938	-1.3637984962	-0.217799609
H	-4.1868224407	-2.1304990826	-0.9900545494
H	-5.2912335127	-0.8986479726	-0.3451426484
H	-4.2933599556	-1.8653497169	0.7545812714
H	-4.4089453186	1.207416679	0.6702328587
H	-2.6782146127	1.5730156866	0.6974962885
H	-3.3435514347	0.3455682342	1.7825065124
H	-2.5485835255	1.1735569614	-1.8155353979

H	-4.2891705829	0.8766881582	-1.7710375854
H	-3.2148330462	-0.3143655527	-2.5144166692
H	-0.543085637	1.3046875804	0.91908656
H	-0.4183176996	1.702002224	-0.7877363511
C	1.1702653156	2.5274742678	0.4349907606
H	1.7827141894	2.1993285535	1.2843977874
C	0.5098975071	3.8727653212	0.7754072934
H	1.8642119368	2.6633058845	-0.4070510083
H	1.2877268653	4.5757436087	1.1001187367
H	-0.15683359	3.7358027349	1.6380980051
C	-0.2779197392	4.4980607014	-0.3818875617
H	-0.6617994443	5.4869372695	-0.1106874502
H	-1.1355871199	3.8818290136	-0.6702620128
H	0.356157713	4.6176467219	-1.2683612893
C	2.9674283711	-2.0990067403	-0.399548296
H	2.3387436177	-2.3977968959	1.6521709172
H	3.3252711486	-0.9840148729	1.4226285979
H	3.4724428695	-3.0619738045	-0.2507068734
C	3.9264675228	-1.1697317446	-1.1688035325
H	2.0907945317	-2.3186817052	-1.0211971412
C	5.3408110801	-1.1320567907	-0.5784620309
H	3.5186857104	-0.1524573618	-1.1920897489
H	3.9856060639	-1.5024310681	-2.2128688928
H	5.795664031	-2.129351926	-0.5868430086
H	5.3388394719	-0.7797954847	0.4585584872
H	5.9915953383	-0.4624571637	-1.1501493253
H	5.9915953383	-0.4624571637	-1.1501493253

TS endo 0525

E(RB3LYP) = -706.410009281 A.U.

First frequency = -513.4229 cm^{-1}

H	-2.1376201641	-0.4861806128	-2.2354922339
C	-1.5306578998	-0.9080829485	-1.4395245466
H	-0.7835049685	-1.6091765573	-1.7911209908
C	-2.045815908	-1.0128197629	-0.148792231
C	-1.1785165703	-1.4736393254	0.8670748517
C	0.1089074458	-1.9140759695	0.6179737888

H	0.7574569904	-2.1511463016	1.4558856102
H	0.3474485199	-2.4401653009	-0.2982576612
C	1.1799011302	-0.1990291201	-0.4860856663
H	1.4144171367	0.1629412297	0.5076537267
C	2.2639141459	-0.9837770397	-1.2017423069
C	0.2144314642	0.4968162182	-1.212250553
H	0.3101032655	0.4797965044	-2.2979021088
C	-0.4409115187	1.7319287366	-0.6410803707
C	-3.4919600752	-0.5658621308	0.1610311059
H	-1.4611599979	-1.3197358087	1.9034576708
C	-4.438212703	-1.6115591893	-0.4798868471
C	-3.8234500529	0.8230806029	-0.4245615085
C	-3.7866907544	-0.5160610546	1.6723104099
H	-3.6547248436	-1.493516417	2.1465254569
H	-4.8249842825	-0.2094771373	1.8359826067
H	-3.1424920343	0.2052440695	2.1861852656
H	-4.8838112982	1.050050534	-0.2673746808
H	-3.6358194214	0.8765734053	-1.5004913952
H	-3.2364056562	1.6060557264	0.0619692501
H	-4.2344763423	-2.6128293859	-0.0865637237
H	-4.3062164993	-1.6460729846	-1.5657053822
H	-5.486474358	-1.3673229694	-0.2703903918
H	-0.7227177521	1.5357054633	0.4009114988
H	-1.3720729099	1.9341741996	-1.1768059172
C	0.4305825221	3.0070372678	-0.7298290457
H	0.6743284574	3.1858571216	-1.7858329747
C	1.7324541178	3.0130272922	0.0858981539
H	-0.1864532064	3.8595615258	-0.4119258004
H	2.2675158165	3.947127565	-0.1283697099
H	2.3867518999	2.2035224459	-0.2573684398
C	1.5224460308	2.8979592992	1.599526614
H	1.0509272434	1.9494551337	1.8766267209
H	0.8758244296	3.7026202922	1.9689152312
H	2.4742359849	2.9610854515	2.1373130234
C	3.3504719659	-1.5695126357	-0.288417236
H	2.7514392162	-0.3291360012	-1.9396487969
H	1.8058116476	-1.7904896643	-1.7936429521
H	2.8925009863	-2.2209632863	0.4662919024

C	4.2079814277	-0.5067198477	0.412503733
H	4.0087926969	-2.2131189562	-0.886803076
C	5.3013321122	-1.1153794934	1.295030491
H	3.5712175344	0.1455047921	1.0232079108
H	4.6639135924	0.1428835349	-0.3474116449
H	5.9779228481	-1.7459798583	0.7068615718
H	4.8671934697	-1.743374477	2.0815316422
H	5.9041117239	-0.3414730335	1.7812033834
H	5.9041117239	-0.3414730335	1.7812033834

TS endo 0526

E(RB3LYP) = -706.411186526 A.U.

First frequency = -531.6372 cm^{-1}

H	-1.3691195008	0.3758394161	-2.1455040739
C	-0.9707076668	-0.3820488857	-1.4813239169
H	-0.3159100159	-1.0893590518	-1.9741923574
C	-1.6430413559	-0.7385162222	-0.3176652966
C	-1.0071661782	-1.6519037743	0.5541390875
C	0.1846936475	-2.2858674161	0.2404530882
H	0.6642717096	-2.9105188325	0.9884142998
H	0.3746837799	-2.5908119062	-0.7822831573
C	1.7129192429	-0.7180454593	-0.2068925488
H	1.9689997632	-0.7220875238	0.8487830808
C	2.6502322173	-1.4731785642	-1.1327410356
C	1.0391509713	0.4109517061	-0.6736554001
H	1.228467972	0.7312434767	-1.6968194112
C	0.62891259	1.4814270377	0.3074374568
C	-2.9835125302	-0.1033433694	0.1139251922
H	-1.3795097515	-1.7390576969	1.5724705815
C	-3.9896934251	-1.2556609862	0.3554624817
C	-3.5792147329	0.8129125537	-0.9709948139
C	-2.8437636154	0.7163114625	1.4156661117
H	-3.8248880341	1.077181128	1.7450511535
H	-2.2017462587	1.5869769108	1.2635153654
H	-2.4188094028	0.1221245187	2.229603819
H	-2.9482920514	1.6848498795	-1.1673144775
H	-4.5559504547	1.1855844528	-0.6449879839

H	-3.7225062375	0.2766756923	-1.9143431641
H	-4.9699499942	-0.8540085427	0.6371003783
H	-3.6578267487	-1.9220433459	1.1566741629
H	-4.1137341295	-1.8590016665	-0.5495774322
H	1.5253693589	1.8261899909	0.8464221477
H	-0.0134992761	1.0250728547	1.0739217174
C	-0.0626084756	2.6955845302	-0.3142207477
H	0.5616791836	3.091700263	-1.1279158763
C	-0.3470647823	3.8175954419	0.6898369215
H	-1.0004164608	2.3773894366	-0.7826723219
H	0.601710293	4.1727415648	1.1143888396
H	-0.9216652082	3.4153331604	1.5350476511
C	-1.1083660398	4.9916248522	0.0683546777
H	-2.0786443117	4.6652487201	-0.3236259546
H	-0.5468521078	5.4285601113	-0.7654141664
H	-1.2935752073	5.7857657561	0.7988873985
C	3.2906245277	-2.7553209514	-0.5705012345
H	3.4548985541	-0.7896510532	-1.4383999402
H	2.1179088362	-1.7192203635	-2.0633014083
H	2.5304913724	-3.536250542	-0.4586853015
C	4.0255067574	-2.5855932297	0.7697145714
H	4.0029659602	-3.1307772332	-1.3173931889
C	5.117545577	-1.5107615968	0.7518965847
H	4.4696451392	-3.5507423863	1.0441903114
H	3.3016672651	-2.3560232745	1.5619942166
H	5.6652358684	-1.4868547745	1.6994964931
H	4.6962313372	-0.5133717809	0.5895088655
H	5.8426902764	-1.6986513537	-0.0486233028
H	5.8426902764	-1.6986513537	-0.0486233028

TS endo 0534

E(RB3LYP) = -706.408768125 A.U.

First frequency = -512.4960 cm⁻¹

H	-1.7799481012	-0.4606048464	-2.2536144404
C	-1.308582012	-0.8912592206	-1.3747595472
H	-0.4640112605	-1.5290301111	-1.6053188445
C	-2.049716089	-1.0935702832	-0.2123770343

C	-1.3608237086	-1.5596240271	0.9296720015
C	-0.0233542044	-1.9120343208	0.9127402468
H	0.4683051931	-2.1586231114	1.8486898176
H	0.4174123622	-2.3733409939	0.0371409044
C	1.1286901782	-0.085596747	0.1090372307
H	1.165586432	0.2440685787	1.1428488086
C	2.3739169169	-0.7667885015	-0.4272483467
C	0.2727652006	0.5941070182	-0.7566198765
H	0.5655073641	0.6339369807	-1.8056829679
C	-0.5522478282	1.763404689	-0.2733972096
C	-3.5544889444	-0.7465140938	-0.1664071111
H	-1.8428435598	-1.4788452807	1.8985737428
C	-4.2919481632	-1.8050596669	-1.023895615
C	-3.8593996589	0.6529238958	-0.7412738534
C	-4.1322692733	-0.7994094457	1.2607102485
H	-4.0278259587	-1.7932246821	1.7069684079
H	-5.2007637645	-0.5616722847	1.2353367045
H	-3.6460224635	-0.0732772825	1.9207039302
H	-4.94282702	0.8118396441	-0.7803338306
H	-3.4759397896	0.7776767364	-1.7577554714
H	-3.4267098617	1.4380733817	-0.1160640196
H	-5.374627291	-1.6319547058	-1.008751339
H	-4.1010121503	-2.8142164798	-0.6445593127
H	-3.9552883675	-1.7702857635	-2.064604252
H	-0.9790572976	1.515882834	0.7081373964
H	-1.3966479369	1.9205427686	-0.9492423967
C	0.2270500007	3.0938750959	-0.1776057757
H	0.6471040224	3.3345929389	-1.1647464391
C	1.3475116455	3.1388118758	0.8669916568
H	-0.4941736514	3.8930074055	0.0453047061
H	2.1139615198	2.3966273262	0.6172558533
H	0.9425854232	2.8416558302	1.8445327762
C	1.9938159775	4.5232477643	0.9761169982
H	1.2581434999	5.2830762461	1.2641320483
H	2.4260743743	4.831721828	0.0171007511
H	2.7957038446	4.5356009516	1.7216613417
C	3.2693913257	-1.3932726586	0.6484053948
H	2.9577326333	-0.0271016353	-0.9918032915

H	2.0935001614	-1.5353029131	-1.1652425779
H	3.5554129449	-0.6132579367	1.3687361456
C	4.5375188138	-2.0655286071	0.1002657525
H	2.6934041385	-2.1334563774	1.214440861
C	5.5310729549	-1.0999119451	-0.5565235664
H	4.2494719292	-2.8423581648	-0.6215618081
H	5.0407744239	-2.5883934542	0.9233977886
H	5.1092546718	-0.622204837	-1.4464760439
H	6.4428651487	-1.6210931471	-0.8659007807
H	5.8212905397	-0.3041536395	0.1395708445
H	5.8212905397	-0.3041536395	0.1395708445

TS endo 0538

E(RB3LYP) = -706.409568041 A.U.

First frequency = -530.6664 cm^{-1}

H	-1.2053591174	-0.3536168692	-2.1109477858
C	-1.0336805343	-0.9716221881	-1.2379261426
H	-0.4664057903	-1.8692165361	-1.4476129671
C	-1.8977297755	-0.9264713442	-0.1473060133
C	-1.5472135161	-1.6775784911	0.9963454762
C	-0.4267922821	-2.4947812728	1.0370603912
H	-0.1492268132	-2.9712732863	1.9737361587
H	-0.1442144466	-3.0586368287	0.1554154961
C	1.3488274424	-1.2726995335	0.5580287202
H	1.4317872968	-0.9999915455	1.6085237884
C	2.2835955266	-2.3746250645	0.0999419789
C	0.9462707524	-0.2609099045	-0.3201572646
H	1.3384210862	-0.2893757502	-1.3344854585
C	0.5649327374	1.0984922403	0.2180075694
C	-3.1512210398	-0.0246081764	-0.1013628433
H	-2.0665355572	-1.4762874192	1.9297553549
C	-3.2846509605	0.8681392399	-1.3481652338
C	-3.1814632841	0.8931788084	1.1419345218
C	-4.380021458	-0.965701514	-0.0474132523
H	-4.354156422	-1.5996206159	0.8442269732
H	-4.4045432539	-1.6223751467	-0.9230659518
H	-5.3101321054	-0.3856259498	-0.0264122327

H	-2.3492294967	1.60238106	1.1342547094
H	-3.133223929	0.3292310796	2.0770998991
H	-4.1122201735	1.4711717055	1.1575074337
H	-2.4467854466	1.5658419233	-1.4376540308
H	-4.2028379683	1.4609756244	-1.2821452779
H	-3.3395189875	0.2768354517	-2.2673403458
H	1.3250478888	1.4271375103	0.9401126336
H	-0.360123614	1.000622032	0.8007726984
C	0.4105153833	2.1656673265	-0.8704870121
H	1.3889226869	2.3283418155	-1.345113521
C	-0.1413184994	3.5092526647	-0.3738996499
H	-0.2455947057	1.7766981931	-1.6575846679
H	-1.1449330705	3.3542929642	0.0449347617
H	-0.2730413569	4.1762217555	-1.2355060611
C	0.7435744389	4.203419394	0.6676888162
H	0.8171225741	3.6193666855	1.5905343827
H	0.3455619181	5.1883215652	0.9327629592
H	1.7610537207	4.3456357879	0.2848473492
C	3.7933662463	-2.0730986523	0.2363683509
H	2.0663716447	-2.6082016902	-0.9523881771
H	2.0854157652	-3.2953611802	0.6630762146
H	4.0308491425	-1.899221191	1.2950163105
C	4.3333143432	-0.8996756949	-0.6082946454
H	4.3262929769	-2.9913136077	-0.04200777
C	4.3489197556	0.4487859514	0.1203180066
H	3.7452261962	-0.8155240827	-1.5315677236
H	5.3571529233	-1.1321293236	-0.926746714
H	3.3525739661	0.7270543722	0.4689412489
H	4.7133869457	1.2501571891	-0.531493215
H	5.0066117732	0.4070200946	0.9962076745
H	5.0066117732	0.4070200946	0.9962076745

TS endo 0546

E(RB3LYP) = -706.410181250 A.U.

First frequency = -535.6226 cm^{-1}

H	-1.7016429583	-0.2057170628	-2.1111869547
C	-1.1636565405	-0.7266461286	-1.3278225739

H	-0.4592329897	-1.4594690787	-1.7008844514
C	-1.7076199205	-0.8596052078	-0.054417031
C	-0.9022190651	-1.4527362601	0.9440013655
C	0.3399903317	-2.0078899569	0.6792560894
H	0.9433353047	-2.3666381962	1.5081121028
H	0.5033717742	-2.5377705532	-0.2522069292
C	1.6152730159	-0.4430070773	-0.293280087
H	1.9570920022	-0.1693412994	0.700748819
C	2.5530784662	-1.3018242732	-1.1241018195
C	0.7615502875	0.459775636	-0.9282125315
H	0.8319715988	0.5492014197	-2.0110139744
C	0.2883275306	1.6811916469	-0.1780857857
C	-3.0903526447	-0.2940650455	0.3384732072
H	-1.193755633	-1.3278670995	1.9845251793
C	-2.9814798667	0.8171732261	1.4056740534
C	-3.9235443229	-1.463444305	0.918855004
C	-3.8609588952	0.272538587	-0.8681947387
H	-3.9922237889	-0.4814954987	-1.6506113391
H	-3.3572410325	1.1378438527	-1.3092348056
H	-4.8555587562	0.6024231608	-0.5502314816
H	-4.9286144078	-1.119407085	1.1892135191
H	-3.460132188	-1.8839366532	1.8158874991
H	-4.0232015005	-2.2705600102	0.1859281958
H	-2.4649345839	1.6932999472	1.0068594693
H	-2.4390804113	0.480964713	2.2937938729
H	-3.9800831122	1.1345164773	1.7271984436
H	1.171877718	2.2148783248	0.1998211214
H	-0.2605457612	1.3538724335	0.7163660063
C	-0.5670524525	2.6430019776	-1.0072855165
H	-0.0192306372	2.9111338553	-1.9223059201
C	-0.9728294662	3.9312985179	-0.2747403745
H	-1.4673927613	2.114999543	-1.3380951979
H	-1.4907428825	3.6738513085	0.6588896652
H	-1.7065229207	4.4686532691	-0.8889747214
C	0.1975953299	4.8710236322	0.0384077994
H	0.918593578	4.4105100763	0.7212516228
H	-0.1525588186	5.7966243038	0.5069055264
H	0.7365296983	5.1429232382	-0.876757039

C	3.4514821809	-2.2786250243	-0.3494405201
H	3.2035605181	-0.6382594851	-1.7139948297
H	1.9639302845	-1.8608244227	-1.8663775672
H	2.8397871168	-2.9927819269	0.2145250225
C	4.4425782463	-1.6003001028	0.6052521474
H	4.0189210169	-2.876077261	-1.0756514397
C	5.367968165	-2.6016863045	1.3027028948
H	3.8971150916	-1.0251018887	1.3636963929
H	5.0418955133	-0.8707158224	0.0434671362
H	6.0679190843	-2.1005747466	1.9791650702
H	5.9565849471	-3.1693534859	0.572880611
H	4.7921873754	-3.3236553965	1.8932664717
H	4.7921873754	-3.3236553965	1.8932664717

TS endo 0548

E(RB3LYP) = -706.408111397 A.U.

First frequency = -532.7275 cm⁻¹

H	-1.5504820659	-0.2376488584	-2.2781253302
C	-1.0970584384	-0.7066960618	-1.4121833743
H	-0.1968346955	-1.2634967834	-1.6477464329
C	-1.8780776519	-1.0805776924	-0.3182579442
C	-1.2068951093	-1.5889429656	0.8144411887
C	0.161611562	-1.793272674	0.8526350656
H	0.628320234	-2.0726711379	1.7925481279
H	0.6929071227	-2.1318295505	-0.0284999233
C	1.1357206487	0.195488385	0.233226091
H	1.128154354	0.4481740875	1.2896044163
C	2.4444590272	-0.3239669112	-0.3283960099
C	0.2233458936	0.8529846582	-0.5976084846
H	0.543732678	1.049891213	-1.6205791617
C	-0.7599644056	1.8468630716	-0.0210623437
C	-3.3996724326	-0.8317089051	-0.2446137737
H	-1.7549622557	-1.6562810614	1.751418247
C	-4.0845990339	-2.2123893613	-0.0949026083
C	-3.9490331713	-0.1616039013	-1.5169861763
C	-3.7925914467	0.0494067866	0.9636162268
H	-4.8826522592	0.149085908	1.0171179163

H	-3.3668145192	1.0521965011	0.8773180302
H	-3.4567356944	-0.3776970385	1.9123810393
H	-3.5143608819	0.830972611	-1.6749763274
H	-5.0333296678	-0.0359442279	-1.4309993393
H	-3.7542545604	-0.7652583152	-2.4090138036
H	-5.1741979957	-2.099428564	-0.0506310879
H	-3.7599539708	-2.720884697	0.817892667
H	-3.8409292135	-2.8610658718	-0.9425434983
H	-1.0821355611	1.4802995277	0.9615777898
H	-1.6593306141	1.8782867837	-0.6458251152
C	-0.2524869379	3.2992280139	0.1283533607
H	0.0186517054	3.6915144784	-0.8617866304
C	0.9224590237	3.5220150801	1.1036165486
H	-1.1105308826	3.8978869674	0.4604492592
H	0.8655224046	2.7861586143	1.916253655
H	0.8068660898	4.5030663187	1.5812088847
C	2.3067115889	3.4660873299	0.4478503421
H	3.1043883466	3.6013068018	1.1863417313
H	2.4103778942	4.257910413	-0.3029998836
H	2.4726051	2.5111962418	-0.0546966852
C	3.3866097028	-0.9240104071	0.7222808023
H	2.9756820866	0.4951401265	-0.8372790539
H	2.235994228	-1.0598653206	-1.1188902095
H	3.5353374643	-0.1796013889	1.5160710377
C	4.7548812322	-1.3482018125	0.1687953758
H	2.9084817938	-1.7882831472	1.1994165989
C	4.6886965122	-2.5013923948	-0.839476176
H	5.3978973224	-1.6434757966	1.0075216145
H	5.2417435698	-0.4806466849	-0.2976097283
H	4.1888345468	-3.3742473406	-0.4031730507
H	5.6907462651	-2.8125380703	-1.1520353071
H	4.1362133289	-2.2218583939	-1.7422638027
H	4.1362133289	-2.2218583939	-1.7422638027

TS endo 0554

E(RB3LYP) = -706.410153698 A.U.

First frequency = -538.3312 cm^{-1}

H	-1.0539889303	0.1596220169	-2.1793482834
C	-0.7096117155	-0.4520043063	-1.3536254436
H	0.1252564207	-1.0925541549	-1.6093811819
C	-1.5690226017	-0.8001573906	-0.3163092257
C	-1.0219019202	-1.505349109	0.7793411754
C	0.2861795019	-1.9629282683	0.8049320566
H	0.6668607196	-2.4159930389	1.7155696411
H	0.7423183871	-2.3390545629	-0.1037575969
C	1.6504425949	-0.2181542191	0.4384838762
H	1.7030155225	-0.0906680664	1.5175621618
C	2.8357567827	-0.9105395862	-0.2085222096
C	0.9251154343	0.7355151706	-0.276466367
H	1.2750726527	0.9941044257	-1.2744032326
C	0.1709680393	1.8065835663	0.4737590837
C	-3.0477901388	-0.3577150167	-0.2572306175
H	-1.5964747562	-1.5521439804	1.7018657708
C	-3.9094543461	-1.6353307466	-0.103064703
C	-3.5020597356	0.3579460639	-1.5426909786
C	-3.3266475136	0.5779059038	0.939636031
H	-2.7931997327	1.5247434369	0.8285255931
H	-3.0234396507	0.1294964369	1.8898818921
H	-4.3974724866	0.8021865629	1.0053803261
H	-3.3526970253	-0.2705120148	-2.4262706164
H	-2.9688215014	1.3002216421	-1.7000329566
H	-4.5690526877	0.5952131433	-1.4765826236
H	-3.7382444901	-2.322340174	-0.9380801538
H	-4.9748144198	-1.3779225691	-0.083359218
H	-3.6762731275	-2.1709001855	0.8216107117
H	0.8731160401	2.3076170829	1.1549914942
H	-0.5730423864	1.3240024248	1.1233017253
C	-0.4993850031	2.8528329731	-0.4211115792
H	0.2551998032	3.2828718949	-1.0956031558
C	-1.1951449146	3.9929153199	0.3384619144
H	-1.2275986694	2.3487904267	-1.0650148818
H	-1.9278954008	3.5718009517	1.0397985367
H	-1.771977525	4.591698849	-0.3778265489
C	-0.2371704202	4.9158247863	1.1010227173
H	-0.7770483431	5.7423687086	1.5745062164

H	0.5099784735	5.348351803	0.4252964938
H	0.3016488931	4.3816914858	1.89004376
C	3.5807250945	-1.8944701073	0.7030181677
H	3.5526623943	-0.1465368561	-0.5463114521
H	2.5034778337	-1.41869952	-1.1254861865
H	3.8423064177	-1.374077121	1.6342817669
C	4.8572196344	-2.479174798	0.0798742886
H	2.9151050105	-2.717470085	0.9900316227
C	4.6025667396	-3.3650757806	-1.1453506183
H	5.3840374857	-3.0668293917	0.8422863408
H	5.534919524	-1.6592428265	-0.1951939691
H	4.1640335751	-2.7987436026	-1.9732055447
H	3.9125711861	-4.1814375401	-0.9012238706
H	5.5324435704	-3.8125949812	-1.5109543501
H	5.5324435704	-3.8125949812	-1.5109543501

TS endo 0555

E(RB3LYP) = -706.407852761 A.U.

First frequency = -535.0412 cm^{-1}

H	-1.3740903668	-0.6763574046	-2.081291658
C	-1.060281723	-1.0395174962	-1.1094333557
H	-0.1847056039	-1.6740787131	-1.1459647927
C	-1.9742818286	-1.1781261511	-0.0676291703
C	-1.4670536931	-1.540554934	1.1983910185
C	-0.1193203003	-1.7684565315	1.4252322294
H	0.231982487	-1.919363606	2.4425454484
H	0.4872788979	-2.2568199229	0.6715508898
C	0.9629241504	0.0702549644	0.7754492235
H	0.6746073651	0.5468547276	1.7092033898
C	2.381220461	-0.4800854547	0.7868375386
C	0.3338561544	0.5607256035	-0.3774810912
H	0.8641359471	0.4730976354	-1.322597593
C	-0.604843216	1.7454933014	-0.2798838279
C	-3.4655015571	-0.8019502937	-0.1988754465
H	-2.1162372379	-1.4360558458	2.0646266392
C	-3.8632126274	0.33068909	0.7753038351
C	-4.2965389002	-2.064213901	0.1362693631

C	-3.8349376789	-0.3532195579	-1.6242530508
H	-3.301594903	0.5574629907	-1.916101098
H	-4.9070118334	-0.1372490603	-1.6789441238
H	-3.6129372486	-1.1301372594	-2.3626866309
H	-4.0497872604	-2.8843060883	-0.545798435
H	-5.3686353752	-1.8536399207	0.0464909149
H	-4.1058789311	-2.4105797426	1.1563667723
H	-4.9374775245	0.53448147	0.6996903669
H	-3.3275680897	1.2548648003	0.543548358
H	-3.6503866576	0.0712675263	1.8159602185
H	-1.0783932387	1.7323191051	0.7095789628
H	-1.4169645299	1.6563764042	-1.0095047901
C	0.0613207372	3.1240669825	-0.4984037919
H	0.3947430034	3.1983518204	-1.5429298387
C	1.244627414	3.4612230354	0.43299314
H	-0.7247549655	3.8812688725	-0.3827974228
H	1.1098098833	2.9502761426	1.3945636126
H	1.233518949	4.5348068188	0.6583025223
C	2.6145441052	3.1038113547	-0.1566668207
H	2.8130734963	3.6958893819	-1.0575010817
H	2.6644784045	2.0497819131	-0.4405535302
H	3.4233530539	3.3002946327	0.5554969032
C	2.858053088	-1.1440656304	-0.5118079748
H	2.4975137218	-1.1969300124	1.6107713239
H	3.0568328165	0.3517879196	1.0302501532
H	2.1416873182	-1.9197859439	-0.8115141378
C	4.2562173541	-1.7727336518	-0.4064959894
H	2.8638297392	-0.4064325794	-1.325191404
C	5.3780478046	-0.7584418122	-0.154089754
H	4.4679824611	-2.3158259264	-1.3361637883
H	4.2551080594	-2.5257614286	0.3933964537
H	5.3829003007	0.0195487494	-0.9265917537
H	6.3591940258	-1.2440448939	-0.1629762822
H	5.2669725314	-0.2605321801	0.8142250564
H	5.2669725314	-0.2605321801	0.8142250564

TS endo 0556

E(RB3LYP) = -706.409476977 A.U.

First frequency = $-506.9404 \text{ cm}^{-1}$

H	-1.6082743834	0.0456585578	-2.0634757177
C	-1.1774887012	-0.5723840683	-1.2809643363
H	-0.33679568	-1.1685344301	-1.6140198168
C	-1.9611424261	-0.9894636978	-0.2082967429
C	-1.3216837651	-1.7011315654	0.83260322
C	0.0053654168	-2.0884413573	0.7785216245
H	0.4601135133	-2.5376867717	1.6560621311
H	0.4602099159	-2.3755716939	-0.161807228
C	1.2463996462	-0.1788392497	0.3867623463
H	1.2989773093	-0.0893498124	1.4687899222
C	2.4622887457	-0.7697758306	-0.2998605448
C	0.4063928664	0.6984462894	-0.2943964263
H	0.6997983456	0.9851796688	-1.3024041073
C	-0.4147417712	1.7019386879	0.4794814653
C	-3.4554687645	-0.6053790706	-0.1318506833
H	-1.8332867757	-1.8047454805	1.7840152165
C	-4.0814136471	-0.9252362055	1.2388744354
C	-4.1950772623	-1.4412010061	-1.2060558977
C	-3.6985583081	0.8920504651	-0.4184445624
H	-4.7748892083	1.0931185381	-0.45885531
H	-3.2724360195	1.2076671852	-1.3746163219
H	-3.2689789805	1.5187623621	0.3668358785
H	-4.0466705368	-2.5124843735	-1.0353721649
H	-3.8233017835	-1.208139282	-2.2085874326
H	-5.2720617751	-1.236329844	-1.1844581712
H	-4.0221489751	-1.9920756136	1.475798758
H	-5.1406995601	-0.648264484	1.2346859882
H	-3.5953055271	-0.366400436	2.0455375373
H	-0.9916353776	1.1645415494	1.2435227891
H	-1.1447357713	2.1742725385	-0.1833615166
C	0.4327830819	2.7903274133	1.1722604315
H	-0.2439893846	3.4784809565	1.6982594958
C	1.3372075389	3.5960763635	0.2266597887
H	1.0572683412	2.3191870575	1.9416422973
H	2.0755384481	2.9212368391	-0.225269038
H	1.9091475955	4.3208044631	0.8199111174

C	0.5790268956	4.3361902637	-0.880600355
H	0.0779366896	3.6400878336	-1.5615743104
H	1.2555048187	4.9530701901	-1.4810877582
H	-0.1895080925	4.9952077715	-0.4597354094
C	3.3281459423	-1.6611854285	0.5984738883
H	3.0769586594	0.0540229777	-0.6878658774
H	2.1497263945	-1.3392893683	-1.1898381206
H	3.658989951	-1.0736581232	1.4669504374
C	4.5552765264	-2.2624910328	-0.1035779835
H	2.7148918196	-2.4762197926	0.9984732945
C	5.5932853134	-1.2291098828	-0.556901209
H	4.2215020638	-2.8508850908	-0.9695235506
H	5.0361094737	-2.9742914887	0.5793037466
H	6.474209784	-1.7164744793	-0.9871944632
H	5.9298926284	-0.616355338	0.2876074043
H	5.1904733265	-0.5515231494	-1.316381615
H	5.1904733265	-0.5515231494	-1.316381615

TS endo 0557

E(RB3LYP) = -706.409131198 A.U.

First frequency = -516.8444 cm^{-1}

H	-1.3558787201	-0.3769156662	-2.0154771308
C	-1.1240617706	-0.9628435461	-1.1308069655
H	-0.3940339565	-1.7421538721	-1.3049743697
C	-2.0572305612	-1.0798776181	-0.1028765553
C	-1.6559101057	-1.7510576819	1.0728085198
C	-0.4167510965	-2.3619756439	1.1910960056
H	-0.112759779	-2.772657938	2.1501953324
H	0.020364704	-2.8636937252	0.3358070126
C	1.1614231286	-0.8306347293	0.8010093081
H	1.112634066	-0.5615744565	1.8549142562
C	2.302885179	-1.7551378661	0.4255167004
C	0.6288974066	0.0924618276	-0.104394012
H	1.0733271094	0.1455691844	-1.0941447291
C	-0.0623863845	1.3314510209	0.4183929101
C	-3.4494619617	-0.420880822	-0.2262929368
H	-2.2486795487	-1.6331361434	1.9738590408

C	-3.3741892769	1.0459005958	-0.7010840893
C	-4.2351500543	-0.4422194007	1.098482691
C	-4.2466321759	-1.2390624653	-1.2724588211
H	-3.7560995854	-1.2087714857	-2.2502097249
H	-5.2616305969	-0.8401441071	-1.3862827704
H	-4.322904577	-2.2883736022	-0.9693026895
H	-4.4021005705	-1.4625248524	1.4574611144
H	-5.2172479586	0.0194410691	0.9529026347
H	-3.717925614	0.1183821395	1.8842912104
H	-4.3843767347	1.4327927108	-0.8753121272
H	-2.8192101099	1.1526315382	-1.6371866973
H	-2.8970732385	1.6797312282	0.0504899619
H	-0.7473024181	1.0045464919	1.211077909
H	-0.689580254	1.768561516	-0.363872225
C	0.8717245522	2.4374917842	0.9767749052
H	0.3734551871	2.9268003742	1.8235255574
C	1.2357743191	3.5288947607	-0.0440258662
H	1.7825096974	1.9820050273	1.3841050423
H	1.8619397512	4.2819593566	0.4520417732
H	0.3132839685	4.0484832189	-0.3383607464
C	1.9498255324	3.0347758455	-1.3064106762
H	1.3322535975	2.324653323	-1.8656286288
H	2.8916838989	2.5337870746	-1.0642118834
H	2.179490233	3.8688126326	-1.9779645131
C	3.7031643277	-1.2051178586	0.7730074208
H	2.2457542788	-1.98381941	-0.6468643477
H	2.1984356216	-2.7165478836	0.9432429094
H	3.7392451369	-1.0139372144	1.8540665505
C	4.1267035904	0.0681949902	0.02901345
H	4.4412708838	-1.9956994586	0.5777749057
C	4.2419249099	-0.1008264777	-1.4891196819
H	5.094261292	0.3990974902	0.4274995466
H	3.412922816	0.8670981954	0.2537742947
H	4.9390613001	-0.9075895877	-1.7442132126
H	4.6048952263	0.81676882	-1.9634269565
H	3.2767329148	-0.3424203244	-1.9452284492
H	3.2767329148	-0.3424203244	-1.9452284492

TS endo 0561

E(RB3LYP) = -706.408681568 A.U.

First frequency = -514.7460 cm⁻¹

H	-1.9165050314	-0.439967618	-2.2223648015
C	-1.3258876815	-0.9326789507	-1.4585664643
H	-0.673209134	-1.7050070492	-1.848501707
C	-1.777666235	-1.0028542776	-0.1433094501
C	-0.9037398185	-1.5646983682	0.8152063699
C	0.3304660291	-2.0979316794	0.4933590846
H	0.9968102648	-2.4159325899	1.2884603305
H	0.4839699744	-2.6050229709	-0.4515100446
C	1.4701529065	-0.4299484388	-0.6395033615
H	1.7904728093	-0.0590055795	0.3281133224
C	2.4710979253	-1.2555355759	-1.4228717582
C	0.4998695535	0.3175038512	-1.3080769842
H	0.5338141982	0.3172966571	-2.397230029
C	-0.0359877601	1.5712770587	-0.6592639072
C	-3.1091904663	-0.3777903153	0.3245561468
H	-1.1315691774	-1.4183856971	1.8686548074
C	-3.9778971294	-1.5235292851	0.8993698734
C	-3.8863615821	0.2800801259	-0.8298428813
C	-2.9059218722	0.6895518463	1.424847579
H	-3.8768882079	1.0391404347	1.7936366297
H	-2.3640768655	1.5559314273	1.0370934339
H	-2.3503618524	0.3001489404	2.2822742453
H	-3.3275384413	1.1113276178	-1.2724932967
H	-4.8345211454	0.6815880616	-0.4573824915
H	-4.1176857091	-0.4376228295	-1.6232001226
H	-4.9498936564	-1.1406143327	1.2317348133
H	-3.4924339356	-2.0013058501	1.7556757691
H	-4.1533266588	-2.2949199153	0.1425630673
H	-0.2598858757	1.3380651045	0.3871254628
H	-0.9840634012	1.8720349433	-1.1221816178
C	0.9510247326	2.7510160986	-0.7276812633
H	1.8866569639	2.4649601974	-0.2281509392
C	0.4123432484	4.0484574524	-0.1051677869
H	1.2114538283	2.9353661542	-1.7785555561

H	-0.5200653563	4.3323363322	-0.6126315433
H	1.1255422849	4.8587102007	-0.3036911389
C	0.1648954882	3.9595640045	1.4054395886
H	-0.1503862572	4.9257174485	1.8127570408
H	1.0764615113	3.6558469492	1.9336228402
H	-0.614826474	3.2310554799	1.6494382014
C	3.4396656909	-2.1483233858	-0.6276528014
H	3.0804053699	-0.5667290623	-2.0286649922
H	1.9289003632	-1.8750388921	-2.1531128216
H	2.8900200326	-2.9452805593	-0.1135904452
C	4.3343218535	-1.4033544072	0.3899814871
H	4.0804853919	-2.6542829059	-1.3600389068
C	3.7956165961	-1.382327384	1.8267623658
H	4.5014083493	-0.3747850335	0.0425564627
H	5.3239576011	-1.8760239504	0.4073711866
H	3.6664770886	-2.4029141434	2.2055157859
H	2.8250557986	-0.8845804486	1.8997251719
H	4.4865819555	-0.8638489829	2.5000349081
H	4.4865819555	-0.8638489829	2.5000349081

TS endo 0564

E(RB3LYP) = -706.408425776 A.U.

First frequency = -538.3791 cm^{-1}

H	-1.8818475958	-0.38836174	-2.2228430066
C	-1.4010582105	-0.8852587846	-1.3875640615
H	-0.6352172514	-1.5900854787	-1.6927868537
C	-2.0950978972	-1.0899748981	-0.1929196039
C	-1.377648902	-1.6488414682	0.8854178217
C	-0.0612496857	-2.0653084927	0.7815747733
H	0.4669330382	-2.3748440518	1.6786766989
H	0.3004680901	-2.5230196085	-0.1306382235
C	1.1223107743	-0.2862754796	-0.0810504813
H	1.2857192893	-0.0025611661	0.9534853624
C	2.2440175232	-1.0377353293	-0.7731574161
C	0.2141148871	0.47567414	-0.8245350768
H	0.4285961411	0.5963952292	-1.8863813872
C	-0.5308691966	1.622474565	-0.1768469688

C	-3.5435941784	-0.607277812	0.0341445829
H	-1.8136157759	-1.5911118305	1.8801430004
C	-4.1324846691	0.0926280216	-1.2041139675
C	-3.6586869677	0.3664723936	1.229730839
C	-4.4035146609	-1.8602979749	0.3317487768
H	-5.4516585313	-1.5800880045	0.4893949091
H	-4.0532693453	-2.3790661017	1.2291933425
H	-4.3592621554	-2.5689642502	-0.5015987526
H	-3.282602826	-0.0729879343	2.1575095531
H	-4.7083314691	0.6338662852	1.3963698795
H	-3.1018505742	1.2885040791	1.0451319108
H	-3.5765987029	0.9999335729	-1.4628938718
H	-5.1682976402	0.3869169573	-1.0057189691
H	-4.1360433531	-0.5660905687	-2.0782495678
H	-0.7663559373	1.3369856439	0.8560262829
H	-1.4927932672	1.766686684	-0.6806794394
C	0.1912225084	2.9888565203	-0.1663025265
H	0.3561092564	3.3186151837	-1.2016070073
C	1.5253884794	3.0547443159	0.6054551522
H	-0.5118346963	3.7115799164	0.2675150949
H	1.4975372831	2.3458572332	1.4430902566
H	1.6290421157	4.048495483	1.0587264382
C	2.7595904905	2.786292868	-0.2621567089
H	2.685469541	1.8206844133	-0.7659437235
H	3.6784568275	2.7838066702	0.3335232874
H	2.863600453	3.5565626811	-1.0349895772
C	3.2527196077	-1.6977285757	0.1813495833
H	2.7801552694	-0.3573971121	-1.4497500062
H	1.8153719094	-1.8050273085	-1.4357196846
H	2.7063735288	-2.3204142805	0.8988372968
C	4.1476212206	-0.7066745269	0.9471650123
H	3.8950058159	-2.3808409476	-0.389899308
C	5.2075619449	-0.0286338236	0.0719755866
H	4.6501100699	-1.2424907147	1.7622372678
H	3.5258574902	0.0596124694	1.4278842441
H	5.8711836455	-0.7725128476	-0.3839445197
H	5.8274029534	0.6563909881	0.659800718
H	4.7566396757	0.553735989	-0.7368305333

H 4.7566396757 0.553735989 -0.7368305333

TS endo 0566

E(RB3LYP) = -706.409453117 A.U.

First frequency = -523.4622 cm⁻¹

H -0.5615275651 -0.1404386368 -2.0871384922
C -0.4476630767 -0.7671121019 -1.2104056255
H 0.3530238909 -1.4891620366 -1.2923751604
C -1.5262419803 -1.0339612736 -0.3724454428
C -1.26511597 -1.7604606413 0.8109117775
C 0.0005965138 -2.2056466501 1.1534631723
H 0.1630531941 -2.6496793837 2.1319773823
H 0.6965152497 -2.5386630575 0.3939532743
C 1.3096685263 -0.3776074002 1.2012814028
H 0.8229028088 -0.0990461836 2.1336712112
C 2.6812634193 -1.0066823374 1.4227274632
C 0.9634315807 0.4049056587 0.0940634238
H 1.6733754186 0.4674536682 -0.7278894212
C 0.1064209623 1.6344220164 0.3039521382
C -2.939687547 -0.4603396515 -0.6096913265
H -2.0382834939 -1.798297578 1.5747302139
C -3.8988992762 -1.6619917832 -0.7915224492
C -3.0143725543 0.4099807233 -1.8771418731
C -3.4350450999 0.3943624636 0.5795426422
H -3.4191593869 -0.1592600197 1.5221045394
H -4.4676057282 0.7179541829 0.4057853987
H -2.8208200991 1.2902154847 0.7047380032
H -2.7301160182 -0.1519853281 -2.7723013283
H -2.3644714801 1.2882192054 -1.8035151122
H -4.0388617155 0.7686531437 -2.0210070802
H -3.5866915793 -2.2834904427 -1.6369934304
H -4.9212979177 -1.3139132272 -0.9796756387
H -3.9167506369 -2.296451293 0.0997820726
H -0.7170291162 1.3734470153 0.9797393219
H -0.350669405 1.9465684839 -0.6403449853
C 0.8913631485 2.8112699872 0.9114993432
H 1.3816913046 2.4678296444 1.8313234049

C	0.0239920976	4.0399335586	1.2277141646
H	1.6996778226	3.1008302371	0.2247195812
H	0.6419538516	4.7845106923	1.7457560281
H	-0.762675659	3.7493521757	1.9378744199
C	-0.6175480839	4.6915727367	-0.0030751153
H	0.1435778465	4.9649483074	-0.7434232049
H	-1.1603409239	5.6026900263	0.2690773675
H	-1.3296818488	4.0205978656	-0.4941120573
C	3.6294134667	-1.1370381203	0.2213029984
H	2.5788708847	-1.9929948301	1.8957358642
H	3.1872416099	-0.3823929625	2.1742205287
H	3.7687256775	-0.1546954639	-0.2491548006
C	3.2137601495	-2.1573861696	-0.8443014881
H	4.6168492263	-1.4249021148	0.6068230469
C	4.2617149599	-2.3162301461	-1.9497590394
H	2.2618846364	-1.8567081406	-1.294773643
H	3.0330085863	-3.1285640928	-0.3639423211
H	5.2203037966	-2.653315267	-1.5390055158
H	4.4397676113	-1.3633613836	-2.4613578295
H	3.9455756102	-3.0450985062	-2.7029258665
H	3.9455756102	-3.0450985062	-2.7029258665

TS endo 0574

E(RB3LYP) = -706.409353500 A.U.

First frequency = -522.1185 cm^{-1}

H	-0.8235885372	-0.3497518191	-2.1860924143
C	-0.5622459108	-0.884608171	-1.2806196871
H	0.2871945513	-1.5442429644	-1.3951475951
C	-1.5189235737	-1.1617277112	-0.3084895448
C	-1.0720109122	-1.7565328489	0.8928505907
C	0.2566106102	-2.0672729479	1.1248119554
H	0.5628826353	-2.4102397242	2.1094320561
H	0.8933359849	-2.4044063279	0.3177171137
C	1.3980713237	-0.1411489336	0.8779655864
H	0.9849481597	0.1810585957	1.8315924105
C	2.8365142064	-0.6346915764	1.0008772499
C	0.871456748	0.5053439655	-0.2458658634

H	1.4836803692	0.5440900568	-1.1440710944
C	-0.0556871063	1.6844552738	-0.046163877
C	-2.9950887221	-0.7271703658	-0.4303827583
H	-1.754782199	-1.7889782664	1.7385637594
C	-3.8572329754	-2.0129510837	-0.4042183771
C	-3.2806936231	0.0157592325	-1.7478264933
C	-3.4355123928	0.1892043467	0.7343026386
H	-4.5044939214	0.4159849614	0.6509681975
H	-2.8906248375	1.1369835819	0.718410444
H	-3.2742730222	-0.275899871	1.7105005329
H	-4.3427720883	0.2760910732	-1.8041584011
H	-3.0429260046	-0.600813616	-2.620328227
H	-2.7083734403	0.9464398274	-1.819444844
H	-3.5827371334	-2.6814145837	-1.2266426046
H	-4.9206965191	-1.7655272516	-0.5026733887
H	-3.7241142329	-2.5639838158	0.5317063893
H	-0.7874228878	1.4264383014	0.7285336319
H	-0.6271728101	1.8896777387	-0.9594341225
C	0.6873542747	2.9633103077	0.3769792621
H	1.2434495081	2.7667325349	1.3036888152
C	-0.2494039159	4.1590765524	0.5820636638
H	1.4423634325	3.2151967431	-0.3813869228
H	-1.0039090887	3.8992018029	1.3373922749
H	-0.8041966181	4.3474862597	-0.3473129531
C	0.4876341008	5.4319836155	1.0079145226
H	1.0245335287	5.2788670353	1.9511026536
H	-0.2025575674	6.2702504258	1.1490667482
H	1.2255102733	5.7301373143	0.2542636444
C	3.6685074586	-0.7787448937	-0.2844499305
H	2.8732358141	-1.5741691853	1.5666984399
H	3.3552954359	0.0957553546	1.6394801182
H	3.6416148165	0.1705232255	-0.8333992185
C	3.2773587823	-1.9237742533	-1.2320707909
H	4.7163878156	-0.923269195	0.0115917655
C	3.5045236697	-3.3230541358	-0.6490583011
H	3.864320335	-1.8258566757	-2.1542315266
H	2.2301347533	-1.815037343	-1.535620105
H	3.2461902571	-4.1007114469	-1.3750634583

H	2.9010986718	-3.4980009231	0.2470000718
H	4.5551201445	-3.4622596529	-0.3689758898
H	4.5551201445	-3.4622596529	-0.3689758898

TS endo 0575

E(RB3LYP) = -706.408057261 A.U.

First frequency = -529.6153 cm⁻¹

H	-1.2357428137	-1.245958226	-1.9300018005
C	-1.0189342863	-1.3885139724	-0.8776761548
H	-0.2556946288	-2.1324866374	-0.6892090391
C	-1.9809002159	-1.1258299748	0.0942938957
C	-1.5819222446	-1.2233997037	1.4449692403
C	-0.2944943218	-1.5694763983	1.8188214808
H	-0.0072644556	-1.507991667	2.8651327241
H	0.2683008049	-2.2984290677	1.2469867556
C	1.0765672856	-0.1015926432	0.8237727742
H	0.7993122187	0.6385237992	1.5700737927
C	2.4024924602	-0.7917097743	1.1228266435
C	0.5805748012	0.1230206944	-0.4671084878
H	1.1356685778	-0.2937162585	-1.3029551058
C	-0.1539024881	1.4084706034	-0.7853209689
C	-3.3883477538	-0.5858269551	-0.2361750022
H	-2.2395164312	-0.8160571827	2.209425805
C	-3.6355471911	0.8044459169	0.393038879
C	-4.419636417	-1.5861208955	0.3400811687
C	-3.6315834777	-0.4698053235	-1.7516807728
H	-2.9503781751	0.2488569419	-2.2190460874
H	-4.6532661623	-0.1227266383	-1.9379154676
H	-3.5096494254	-1.433869135	-2.2555590991
H	-4.32287801	-1.6815090185	1.4256559384
H	-4.2814536073	-2.580954477	-0.0956073546
H	-5.4410482785	-1.2539411997	0.1207057919
H	-2.9587893625	1.5520517215	-0.0288550373
H	-3.4940219922	0.7963407316	1.4772098978
H	-4.6632391988	1.1310804962	0.1969336629
H	-0.7551337961	1.7027891227	0.0818158773
H	-0.8599260502	1.2538141738	-1.6084601726

C	0.7939531967	2.5608903019	-1.1898891119
H	1.3693131167	2.2402728119	-2.0692583525
C	1.7701594592	3.0436134935	-0.1063470686
H	0.1819235236	3.4121227939	-1.5203545716
H	2.4514698946	3.7774143822	-0.5556832209
H	2.3970277198	2.2052740152	0.2201088736
C	1.0861811086	3.6788402242	1.1088690781
H	0.4468660248	2.9640400062	1.636484599
H	0.4545054184	4.5226059818	0.8070845017
H	1.8224577442	4.0532918205	1.8275876116
C	2.9499227325	-1.7346300216	0.0322370724
H	2.3230467795	-1.3421476365	2.0676131642
H	3.147048749	-0.0065756468	1.3206809597
H	3.5682389501	-2.5076375774	0.5062212905
C	3.7985967219	-1.0431253321	-1.0526452063
H	2.1163246849	-2.2710046352	-0.4383473118
C	5.1788082511	-0.5974688158	-0.5560691949
H	3.2611875842	-0.1733468269	-1.4478582801
H	3.9296097241	-1.733449616	-1.8956083212
H	5.1021697806	0.1235178993	0.264699625
H	5.7524548552	-0.1202582815	-1.3572300977
H	5.7597763567	-1.4523712726	-0.1911273326
H	5.7597763567	-1.4523712726	-0.1911273326

TS endo 0580

E(RB3LYP) = -706.410125248 A.U.

First frequency = -500.5750 cm⁻¹

H	-1.9359067623	-0.8420938816	-2.1132371673
C	-1.3771589834	-1.1846511015	-1.2474350232
H	-0.716029825	-2.0159015207	-1.4572197364
C	-1.8729606696	-0.9777840951	0.0356654361
C	-1.0502598232	-1.3490629874	1.1247826482
C	0.1665671184	-1.9870710043	0.9660726097
H	0.7965556941	-2.153684235	1.8344602841
H	0.3187400496	-2.6920231134	0.1575686644
C	1.4372637816	-0.6371127386	-0.3871619455
H	1.7236637451	-0.114830686	0.5202382043

C	2.4306585184	-1.6413031904	-0.9391887425
C	0.5574301709	0.0243417234	-1.2399483736
H	0.6290986205	-0.1946437752	-2.3041978858
C	0.0453204628	1.3931761053	-0.8664843536
C	-3.2396107439	-0.2894230061	0.2508101108
H	-1.2903383637	-0.971174964	2.1131920125
C	-3.4778969205	0.1125015196	1.7188694689
C	-4.3307334185	-1.3117272276	-0.1536986682
C	-3.4098518961	0.9796468758	-0.6116843379
H	-4.4297341968	1.365905427	-0.5063651264
H	-3.2432752614	0.7872589713	-1.6749691818
H	-2.7193708667	1.7664787344	-0.2981606781
H	-4.243712743	-2.2281702921	0.4390482433
H	-4.2370863427	-1.5863364337	-1.2089263337
H	-5.3325119645	-0.8947069879	0.0041632785
H	-3.4646154126	-0.7536413843	2.3876547659
H	-4.4596675848	0.5871479576	1.8169832029
H	-2.7262027486	0.8283340371	2.0684693527
H	-0.3727200155	1.3352036581	0.1462253301
H	-0.7771471128	1.6827154147	-1.5289653907
C	1.1315931661	2.4844371147	-0.915397249
H	1.9330794741	2.2284884112	-0.2091188022
C	0.6046123873	3.8939157847	-0.6040907827
H	1.5929552529	2.4836126576	-1.9118539596
H	-0.1731028395	4.1574911984	-1.3341975354
H	1.4177726964	4.6161893866	-0.7514182615
C	0.0451303532	4.0517986172	0.8147876897
H	-0.8398250157	3.4274214313	0.9751340053
H	-0.2450030719	5.0886871568	1.0133210664
H	0.7917487757	3.764217631	1.5645120986
C	3.2860994462	-2.4003141806	0.091069589
H	3.1062984956	-1.1119251388	-1.6261163427
H	1.8986644639	-2.3692815216	-1.5689530999
H	2.6640422188	-3.1152552407	0.6407852253
C	4.0294117024	-1.5110858943	1.1022353003
H	4.0229967028	-3.0000456251	-0.4597860782
C	4.9121453174	-0.4360477004	0.4591134493
H	4.6467363944	-2.1555770959	1.7406646738

H	3.30612968	-1.0326392399	1.7747385939
H	4.3140763198	0.2943039471	-0.0957183331
H	5.6277983287	-0.8803446952	-0.2426047354
H	5.4830331327	0.1118725282	1.2156551399
H	5.4830331327	0.1118725282	1.2156551399

TS endo 0594

E(RB3LYP) = -706.409383430 A.U.

First frequency = -525.8501 cm⁻¹

H	-0.8261175438	-0.7305468036	-2.1724565845
C	-0.6221858682	-1.0515055088	-1.1576985213
H	0.2349336578	-1.7055923464	-1.0725616258
C	-1.6396911536	-1.1322812469	-0.2112384862
C	-1.2691067355	-1.4480978987	1.1143774616
C	0.044680161	-1.669426129	1.4914446087
H	0.2845750638	-1.7829180353	2.5453318961
H	0.7384923761	-2.1634265147	0.8231237245
C	1.1614968414	0.1860074361	0.9120229473
H	0.669221256	0.6974022295	1.7348743314
C	2.5896262154	-0.2310520227	1.2538418512
C	0.7337174753	0.5606768714	-0.3686131705
H	1.4227683655	0.3961240571	-1.1952339343
C	-0.1867522922	1.7507393086	-0.550071127
C	-3.1044803617	-0.7498803058	-0.5107963759
H	-2.0050149728	-1.3098363506	1.9031434121
C	-3.9795969185	-1.9933694635	-0.2203746138
C	-3.3166643512	-0.3488149392	-1.9815663506
C	-3.5905991778	0.4198338642	0.375601922
H	-3.4823445064	0.20185131	1.441518699
H	-4.651081837	0.6219061997	0.1864921136
H	-3.0316671614	1.3346063329	0.1608535689
H	-2.7413258288	0.5445836997	-2.2452420706
H	-4.3737994033	-0.122832795	-2.1558636623
H	-3.0307495536	-1.1541688193	-2.6655009609
H	-5.033968993	-1.7788204254	-0.4302263728
H	-3.9010196738	-2.3035386716	0.8258833859
H	-3.6711706454	-2.8394319911	-0.8429794744

H	-0.9265539592	1.7546219183	0.2571636596
H	-0.7528439633	1.6575450052	-1.4832936043
C	0.558929539	3.1041720306	-0.5882945813
H	1.2982537697	3.0693597513	-1.4000840989
C	1.2640589076	3.5243733397	0.7103069509
H	-0.1624173122	3.885694288	-0.86666496
H	1.8276488668	4.4458333741	0.5156467265
H	2.0063552701	2.7661575248	0.9856550919
C	0.3114277477	3.7631737459	1.8867146382
H	-0.2220085176	2.8506345605	2.1712499938
H	-0.4427004593	4.5179062376	1.6342286881
H	0.853434504	4.1154485577	2.7704572096
C	3.5225517493	-0.6502099339	0.1078959439
H	2.5865940486	-1.0264833884	2.0111956444
H	3.0521572268	0.6335111991	1.7532201353
H	3.5670382635	0.1484810959	-0.6443349454
C	3.1759459922	-1.9765510146	-0.5777278802
H	4.5384864218	-0.7294995045	0.5178384339
C	4.2075785571	-2.381656274	-1.6346284313
H	2.1901280549	-1.9041144824	-1.0495028839
H	3.095418821	-2.7658263286	0.1819350485
H	5.2024112378	-2.4991446796	-1.1899704213
H	4.2855363993	-1.6199519079	-2.4189218682
H	3.941771227	-3.3288239879	-2.1149034989
H	3.941771227	-3.3288239879	-2.1149034989

TS endo 0598

E(RB3LYP) = -706.406931922 A.U.

First frequency = -542.3846 cm^{-1}

H	-1.6493478943	-1.0883730921	-2.0878900312
C	-1.25932112	-1.3046363585	-1.0998615915
H	-0.5021733205	-2.0795545186	-1.0946005408
C	-2.0340351262	-1.0827041922	0.0371891426
C	-1.4188356206	-1.2816693494	1.2916270163
C	-0.1094630227	-1.7164879723	1.4191682305
H	0.3549992492	-1.733086985	2.4016628379
H	0.2898733894	-2.4505221622	0.7291085664

C	1.1510709359	-0.2957585364	0.2350392157
H	1.1915152881	0.3520993803	1.1029714378
C	2.3653853542	-1.1818905993	0.045603019
C	0.4311047166	0.1392322759	-0.8843717507
H	0.7888198004	-0.2349754413	-1.8428698533
C	-0.2515569427	1.5018006857	-0.9769326468
C	-3.4622241442	-0.4996539557	-0.0166722154
H	-1.9157788024	-0.8952081693	2.1785329921
C	-3.5714833956	0.8404516501	0.7457719923
C	-4.4095765661	-1.5290177781	0.6463835196
C	-3.9478505838	-0.2650669682	-1.4585504794
H	-3.9389089849	-1.1900656177	-2.0437166691
H	-3.332908686	0.4748831876	-1.9817558908
H	-4.975647423	0.1123291246	-1.4466925466
H	-4.3676266878	-2.4895093162	0.122645903
H	-5.4451256995	-1.1699120165	0.6230452742
H	-4.138009734	-1.7071465679	1.6911340997
H	-2.9540919183	1.6119215346	0.2794504982
H	-3.2577662386	0.7477635817	1.7890186653
H	-4.6095009659	1.1922651847	0.7441032795
H	-1.283092292	1.3773317605	-1.3195831716
H	0.2471789024	2.0652675334	-1.7780375807
C	-0.2581250275	2.3588828962	0.3026891345
H	-1.0501947063	3.1142564883	0.2124716723
C	1.064087862	3.0894957788	0.604132184
H	-0.5453957547	1.7312151364	1.1540265396
H	1.8978525697	2.3786957755	0.5743671858
H	1.0271418238	3.4782112271	1.6298894118
C	1.3575727678	4.2486812442	-0.3553501643
H	2.2931253888	4.7530273024	-0.0921429094
H	0.5555078818	4.9954745899	-0.3274121495
H	1.4524241228	3.9055596554	-1.3909478583
C	3.6029736757	-0.385591568	-0.4100256122
H	2.1456919552	-1.9540589765	-0.7069823146
H	2.5948876462	-1.7134313671	0.9758508471
H	3.3479123353	0.1544813533	-1.3304303779
C	4.8540967081	-1.2440835689	-0.6524403231
H	3.829256873	0.3841608015	0.3417360099

C	5.4121142049	-1.912900076	0.6092203283
H	5.6335686414	-0.6110767285	-1.095441824
H	4.623061668	-2.0125011853	-1.4032215172
H	6.3377517841	-2.4561876835	0.3928904037
H	4.7044167652	-2.6296244528	1.0378094685
H	5.6355772016	-1.1669863613	1.3810164597
H	5.6355772016	-1.1669863613	1.3810164597

TS endo 0600

E(RB3LYP) = -706.408748940 A.U.

First frequency = -516.0891 cm^{-1}

H	-1.3685553904	-0.8116400225	-2.1157540505
C	-0.9750140295	-1.0765138052	-1.1389061015
H	-0.0617750738	-1.6531863925	-1.1778971534
C	-1.8224724831	-1.1646795355	-0.0384516681
C	-1.235756147	-1.3955001918	1.2256885062
C	0.1253482886	-1.589021313	1.3949304364
H	0.533109036	-1.6463008055	2.4004969223
H	0.699766279	-2.1295535578	0.6520208985
C	1.1513528417	0.2179539065	0.5691365981
H	0.8993387165	0.736890538	1.4900866482
C	2.5740111443	-0.3208200351	0.5373798302
C	0.4634396675	0.6335389515	-0.572732524
H	0.9407921013	0.4890084965	-1.5388777441
C	-0.5051685131	1.7920183222	-0.506300148
C	-3.3422492854	-0.9329753761	-0.1962914724
H	-1.8300967466	-1.2237236719	2.117002228
C	-4.0692149002	-0.8178286551	1.1570141177
C	-3.9159233625	-2.1594242073	-0.9482741729
C	-3.6640892159	0.3390988996	-1.0088471287
H	-3.3372076406	1.2381106887	-0.4802926013
H	-4.7454249073	0.4154899807	-1.1685958075
H	-3.1899133409	0.3336880225	-1.9940815049
H	-5.0018454321	-2.068001956	-1.0698517831
H	-3.7094156196	-3.0838056489	-0.3989951978
H	-3.4678636189	-2.2544452739	-1.9421350564
H	-5.1410664716	-0.6704755517	0.9889018533

H	-3.7042461371	0.0337884873	1.7408136956
H	-3.9536394357	-1.7231954205	1.760963939
H	-1.0909905171	1.7151372668	0.4197319255
H	-1.2189560757	1.7285731272	-1.3320558125
C	0.1704613033	3.1797517079	-0.5726455641
H	0.7503141837	3.251052614	-1.5040925947
C	1.0786989776	3.5337681911	0.6099410858
H	-0.619933793	3.9398377078	-0.6509716587
H	1.9114685535	2.823117977	0.6599753676
H	0.5170163902	3.4112668658	1.5465326075
C	1.6294331262	4.960329334	0.522072027
H	2.2147933323	5.0997600761	-0.3942402195
H	2.2800357191	5.1940672785	1.371267883
H	0.818951485	5.6982008438	0.5091993855
C	2.9700497778	-1.1137616331	-0.7159718533
H	2.7459992226	-0.93559479	1.4282934497
H	3.2659819836	0.5310574909	0.6345285257
H	2.2610991022	-1.9368746977	-0.8799337503
C	4.3941740862	-1.6897813149	-0.6590135968
H	2.8886410441	-0.4636368019	-1.5950828558
C	4.5808822035	-2.8012613569	0.38043811
H	5.104610228	-0.8757220877	-0.4596519145
H	4.6533744329	-2.0834374972	-1.6498700052
H	4.4189879015	-2.4395826944	1.4006812661
H	5.5929356676	-3.2165586666	0.3371115726
H	3.8754837202	-3.6220445304	0.2052327652
H	3.8754837202	-3.6220445304	0.2052327652

TS endo 0604

E(RB3LYP) = -706.409799685 A.U.

First frequency = -539.5640 cm^{-1}

H	-1.1936798175	0.3117591829	-2.0157323941
C	-0.8306806816	-0.3527514876	-1.2402897777
H	0.0577627044	-0.9034378377	-1.5232139142
C	-1.6918502065	-0.8574589262	-0.2713219968
C	-1.1259078128	-1.6219935928	0.7735754382
C	0.212850886	-1.9838823002	0.8042398605

H	0.5973835754	-2.4960362304	1.6814048551
H	0.7194935774	-2.2433173029	-0.1186113482
C	1.4532722064	-0.1327708096	0.6617501766
H	1.4666950158	-0.1074484047	1.7494341887
C	2.7073909042	-0.667483076	-0.0050613175
C	0.680578908	0.8348274676	0.0177778226
H	1.0398008818	1.2125923664	-0.9360363485
C	-0.1939062146	1.7422007992	0.8466646242
C	-3.1999162471	-0.5243409944	-0.2222657137
H	-1.7220292283	-1.7972287424	1.6663956964
C	-3.6719923847	0.2539907907	-1.4643757647
C	-3.576588922	0.2931635338	1.0339316588
C	-3.972095438	-1.8666612756	-0.1919668741
H	-3.7289679121	-2.4541682825	0.6979492698
H	-3.7285976955	-2.4746811488	-1.0692038761
H	-5.0531475696	-1.6853859024	-0.1895370983
H	-3.2591215844	-0.2043479335	1.9547588043
H	-4.6633068771	0.4259829622	1.0869329403
H	-3.1200730695	1.2860063942	1.0120685104
H	-3.2051267255	1.2407300695	-1.5355573215
H	-4.7547527976	0.4097516123	-1.4139884401
H	-3.4543659752	-0.2935043858	-2.3868493461
H	0.4237099086	2.2196653575	1.6207285435
H	-0.9052071151	1.1133446964	1.3989941661
C	-0.9515056623	2.8261358565	0.0696903257
H	-1.6244966794	2.3443245767	-0.6470551638
C	-0.0670825166	3.8333832566	-0.6852860608
H	-1.5905417508	3.3778625201	0.772494804
H	-0.7215179185	4.5410662291	-1.2100103349
H	0.4994939896	3.3156736171	-1.4699426815
C	0.9030291862	4.6111874972	0.2103078829
H	1.6482329904	3.9510498862	0.665577232
H	0.3688443452	5.1181785287	1.0224756451
H	1.4438121722	5.3731902104	-0.3603399897
C	3.4948323049	-1.6850713656	0.8306316998
H	3.3748418911	0.17707987	-0.2351239238
H	2.4431726828	-1.1000881626	-0.9809300396
H	3.6862718888	-1.2474219757	1.8197329478

C	4.8312040651	-2.1084129202	0.202532874
H	2.8842059805	-2.5791497766	1.005558829
C	4.6836759234	-2.8761656062	-1.1164089384
H	5.3756408463	-2.733978001	0.9211372541
H	5.4539210059	-1.2177883938	0.040494477
H	4.2316028588	-2.2581810571	-1.898763244
H	4.0487510963	-3.760395327	-0.9854651329
H	5.6558162275	-3.2158323494	-1.4881169848
H	5.6558162275	-3.2158323494	-1.4881169848

TS endo 0622

E(RB3LYP) = -706.409835254 A.U.

First frequency = -536.5234 cm^{-1}

H	-0.8087363256	0.5972481851	-1.7986002055
C	-0.6529360866	-0.2622491109	-1.1577868307
H	0.1987496809	-0.8642618989	-1.4371769856
C	-1.7000926197	-0.8157549247	-0.4304048166
C	-1.3958607681	-1.8602033061	0.4704543818
C	-0.1193258936	-2.3974329168	0.5921448532
H	0.0672437894	-3.1389948892	1.3648078423
H	0.4849059273	-2.5344368356	-0.2980437248
C	1.2669956469	-0.824427125	1.1267860318
H	0.996757808	-0.9618936043	2.1723967485
C	2.5942609647	-1.4748486816	0.7606351662
C	0.8261942835	0.3734575277	0.5547789156
H	1.4179954694	0.8290788806	-0.2320341075
C	-0.0473368479	1.2814579392	1.3867544422
C	-3.1427076169	-0.2623658001	-0.4746358751
H	-2.1372921765	-2.1311033247	1.2186784826
C	-4.0858168894	-1.4406922915	-0.8209330824
C	-3.3271712653	0.8146163441	-1.5599496597
C	-3.5751560179	0.34036769	0.8808265183
H	-3.4553287167	-0.3728396393	1.7013612038
H	-4.6310329227	0.632596597	0.8461196626
H	-2.9900635073	1.2322895859	1.1202045883
H	-4.3767823347	1.1246011455	-1.5986986473
H	-3.0517859176	0.4375915238	-2.5499275123

H	-2.7319797218	1.709799169	-1.3572834035
H	-5.1219716061	-1.091031702	-0.8957653394
H	-4.0517766519	-2.2253611395	-0.0598603648
H	-3.8069213799	-1.8928521495	-1.7781651095
H	0.4934900343	1.5415280067	2.3108139827
H	-0.9175067157	0.6981713685	1.716553054
C	-0.5019444351	2.580203361	0.7133735936
H	-1.0266548215	2.3424759051	-0.2182968957
C	0.635413608	3.5648575193	0.41186248
H	-1.2357017454	3.0797145381	1.3606268384
H	1.3742111066	3.0899794722	-0.2461136083
H	1.166502513	3.7988652231	1.3446631553
C	0.1377584784	4.8586552583	-0.2388599928
H	0.9610996027	5.5501072383	-0.4456967013
H	-0.5782628881	5.3759122423	0.4101505841
H	-0.3702206878	4.6506974961	-1.1877139325
C	3.0298163793	-1.3512949671	-0.7062635396
H	2.5673730432	-2.5399727667	1.0291733414
H	3.3689176022	-1.0315359037	1.4021708611
H	2.2329999147	-1.7294525524	-1.3586705439
C	4.3272629972	-2.1083796375	-1.0322776661
H	3.1612471283	-0.2932191458	-0.967583934
C	5.5677437199	-1.5690417872	-0.3106836872
H	4.4965439484	-2.0625163056	-2.1154947124
H	4.1950126093	-3.1716212544	-0.7893520334
H	6.4717221162	-2.0959710104	-0.6327974318
H	5.4904256496	-1.6843496747	0.7749817919
H	5.7101734622	-0.5025178958	-0.521037612
H	5.7101734622	-0.5025178958	-0.521037612

TS endo 0623

E(RB3LYP) = -706.409416538 A.U.

First frequency = -541.2770 cm^{-1}

H	-1.2821283709	0.4742160046	-2.0111241489
C	-0.9401164017	-0.2792089154	-1.3110359578
H	-0.0884370803	-0.8455484997	-1.6669138849
C	-1.8097109299	-0.831216975	-0.3754627705

C	-1.2663954217	-1.7201257679	0.5789391333
C	0.0518643432	-2.1512015597	0.5452226933
H	0.4224957506	-2.7633822775	1.3622631429
H	0.5274830785	-2.3489079744	-0.4088441123
C	1.3889621692	-0.3604972998	0.5377497673
H	1.4333258994	-0.4454055291	1.6214651907
C	2.5945288255	-0.8886792681	-0.2188660791
C	0.6497449675	0.7028786229	0.0171673584
H	1.0053761534	1.1602604152	-0.9025654159
C	-0.1611025928	1.5590155462	0.9577149858
C	-3.2972798054	-0.428814977	-0.2614650373
H	-1.8554285528	-1.9502088462	1.4640598573
C	-4.1377017838	-1.726978842	-0.347576573
C	-3.7480571674	0.4926182581	-1.4099712547
C	-3.6108472976	0.2771052262	1.0770577305
H	-3.3066567632	-0.3257109618	1.9374483502
H	-4.6880342309	0.4596740776	1.1649501974
H	-3.1025783823	1.2423668215	1.1445575062
H	-4.8202681806	0.6967880465	-1.3213583335
H	-3.5742649714	0.0299775654	-2.38659699
H	-3.2314625741	1.4567533044	-1.3927467652
H	-5.2076860223	-1.4930720952	-0.3029840577
H	-3.9098029417	-2.4120834844	0.4739264392
H	-3.9412524294	-2.2553274468	-1.2860769174
H	0.4935367607	1.9178407693	1.7646411197
H	-0.8958783533	0.9116512397	1.4551954799
C	-0.8719705724	2.7571770274	0.3163318211
H	-1.572715309	2.3897424865	-0.4406385723
C	0.0540690802	3.7997622617	-0.3335522694
H	-1.478489713	3.2566556971	1.084012403
H	-0.5697077773	4.5888623275	-0.7724808592
H	0.593060784	3.3453065149	-1.1747367343
C	1.0625100604	4.4317816096	0.6317655094
H	0.5554920781	4.8718300626	1.4985529072
H	1.6352141199	5.2257564353	0.1415041252
H	1.7787419839	3.6936791944	1.0066940215
C	3.3706724567	-1.9921886801	0.5106611183
H	3.2717395996	-0.0483470012	-0.4226940841

H	2.2825150205	-1.2548532604	-1.2100412328
H	3.7048014331	-1.606120835	1.4844375039
C	4.5839426297	-2.5276474819	-0.2652106495
H	2.6959082905	-2.8270611572	0.7298619992
C	5.698346882	-1.497790822	-0.4850449371
H	4.2466687959	-2.9155382207	-1.2364201939
H	4.995798466	-3.3875336043	0.2780773974
H	5.3650322714	-0.6619901161	-1.1083328453
H	6.5630487291	-1.9511149266	-0.9805135987
H	6.0408324342	-1.0820761467	0.4698756044
H	6.0408324342	-1.0820761467	0.4698756044

TS endo 0624

E(RB3LYP) = -706.410208941 A.U.

First frequency = -536.2358 cm^{-1}

H	-0.8051516707	0.1918023791	-1.8876572429
C	-0.6361225245	-0.4801393878	-1.0546482318
H	0.2650573888	-1.0683295578	-1.1449864424
C	-1.6887994137	-0.9187043253	-0.2600037537
C	-1.3769991919	-1.694486733	0.8786742902
C	-0.0818753134	-2.097447917	1.180790315
H	0.1020991915	-2.6183379276	2.1169904441
H	0.5810376264	-2.3975399908	0.3767301493
C	1.1778579247	-0.3448146552	1.3800931156
H	0.8514817588	-0.2464033242	2.4139805651
C	2.5569126915	-0.9749693221	1.2415804725
C	0.7082851105	0.6453267096	0.5117431314
H	1.3233048921	0.9302902796	-0.3349030962
C	-0.2542692281	1.6747687027	1.051222114
C	-3.157410873	-0.4982977199	-0.496839591
H	-2.1437101731	-1.8295100694	1.6382441679
C	-3.3465775623	0.2562470113	-1.826095145
C	-3.6977112642	0.3895846838	0.6465707775
C	-4.0091787934	-1.7895324993	-0.5706718263
H	-3.6514821785	-2.445507973	-1.3708249573
H	-5.0580920624	-1.5433291473	-0.7721851441
H	-3.9726153066	-2.3551026565	0.3645991429

H	-3.5803496269	-0.0889260382	1.6230995038
H	-4.7655898016	0.5887724879	0.5000902361
H	-3.1803620387	1.3520977498	0.6781955155
H	-4.4091856102	0.4702323721	-1.9820511593
H	-2.9946660297	-0.3366676309	-2.6761807686
H	-2.818302215	1.2140210268	-1.8369819823
H	0.2226438487	2.1886464905	1.8991312066
H	-1.1106662029	1.1432244012	1.4874413823
C	-0.7515495981	2.7269328091	0.0522314307
H	-1.3485136157	2.2328207248	-0.7204242672
C	0.3489542282	3.5555237175	-0.632361601
H	-1.4309537527	3.4103784455	0.5796318396
H	-0.1310973591	4.2820274435	-1.300273574
H	0.9497257026	2.9073617666	-1.2832338175
C	1.2741155192	4.2948414266	0.3399505534
H	1.8581673583	3.596279907	0.9478549221
H	0.6999130296	4.9300302184	1.0246365054
H	1.9813870872	4.9358952413	-0.1962844074
C	3.0729906184	-1.1870839798	-0.1872620834
H	2.5732765925	-1.9389423593	1.7678184258
H	3.2778071364	-0.3390092825	1.7782984376
H	2.3675705512	-1.8075584916	-0.756025142
C	4.4557095249	-1.8482090786	-0.2252910995
H	3.1243925903	-0.2258618291	-0.7144871512
C	4.9797636119	-2.0524445271	-1.6494314823
H	4.4081893643	-2.8156490957	0.292723763
H	5.1652985522	-1.2331314775	0.3446926852
H	4.3028761572	-2.6891231671	-2.2306423381
H	5.9667659957	-2.5260745039	-1.6512120821
H	5.0671871939	-1.0963071458	-2.1780707161
H	5.0671871939	-1.0963071458	-2.1780707161

TS endo 0626

E(RB3LYP) = -706.409441298 A.U.

First frequency = -531.8463 cm^{-1}

H	-1.2313695214	0.0747528784	-2.1089553937
C	-0.8816337271	-0.5336930145	-1.2832949574

H	-0.150213258	-1.2782896693	-1.5726444086
C	-1.6738816897	-0.7347036104	-0.1570740526
C	-1.1092382573	-1.4493003212	0.9239175829
C	0.1470830757	-2.0279738058	0.8774420995
H	0.5511598019	-2.4763484247	1.7800198729
H	0.5109666925	-2.468698955	-0.0432367381
C	1.6276967934	-0.4059960353	0.3230269619
H	1.7321728733	-0.1892581194	1.3837786796
C	2.728025009	-1.2502156304	-0.2972985514
C	0.9566446967	0.5344651565	-0.4583341171
H	1.2764668955	0.6291137105	-1.4952592395
C	0.3800775169	1.7840395235	0.1702687615
C	-3.0933538091	-0.1470346418	-0.0026036942
H	-1.6112641801	-1.4081520398	1.8872705892
C	-3.5005500033	0.742007011	-1.1909202536
C	-3.2505693252	0.6836381307	1.2904926202
C	-4.0738666457	-1.3445529419	0.0578764687
H	-4.0054102037	-1.9491927494	-0.8523002335
H	-5.1070133503	-0.9918145633	0.159421412
H	-3.8521114083	-1.9961155979	0.9085717139
H	-2.5833481398	1.5480809641	1.2890388972
H	-3.040807417	0.0967091495	2.1885679731
H	-4.2783053343	1.0540960289	1.3768488241
H	-3.4701187276	0.1937155532	-2.1375351834
H	-2.8528009025	1.618647115	-1.2814230541
H	-4.5251158785	1.1018296249	-1.0502736822
H	1.142038195	2.2371842926	0.8232507615
H	-0.446230762	1.5013429908	0.8345292505
C	-0.0636183817	2.834057512	-0.855574604
H	0.7504454645	2.973859199	-1.5800032866
C	-0.4220302923	4.2029350439	-0.2591855137
H	-0.9137667953	2.4471950632	-1.4301754347
H	-0.6295348926	4.9000536003	-1.0811019618
H	0.4552598537	4.6051807752	0.2660295818
C	-1.6199350839	4.1860444603	0.695862341
H	-2.5089776587	3.7728914643	0.2061643204
H	-1.8673781537	5.1961486847	1.0385793417
H	-1.4189000182	3.5789990012	1.5842612815

C	3.444102977	-2.1932891826	0.6773627248
H	3.4682005951	-0.5738884166	-0.7459136704
H	2.3218708284	-1.8324076234	-1.1396881215
H	3.8592912777	-1.5998361577	1.5046518851
C	4.5670075206	-3.0247753443	0.0375716296
H	2.7152178096	-2.8752612741	1.1280001147
C	5.7560741865	-2.1999349133	-0.4689273635
H	4.1502862648	-3.6142154662	-0.7909074116
H	4.9276643653	-3.7524756753	0.7755369633
H	6.1800275218	-1.5893207618	0.3369077083
H	5.4684762646	-1.523061494	-1.2796236481
H	6.5521134586	-2.8476732746	-0.8503633768
H	6.5521134586	-2.8476732746	-0.8503633768

TS endo 0632

E(RB3LYP) = -706.408161188 A.U.

First frequency = -512.6536 cm⁻¹

H	-1.9052257683	0.2029141071	-1.9502482694
C	-1.3197577015	-0.4957058218	-1.3636118336
H	-0.6192421731	-1.0745364829	-1.9541378056
C	-1.8130374397	-1.0114024456	-0.168089979
C	-0.9474364007	-1.8302148063	0.5928032033
C	0.3206465277	-2.1867256517	0.1731406365
H	0.9729756459	-2.7285467825	0.8500917413
H	0.5305009693	-2.3465291062	-0.8775050559
C	1.4217691132	-0.2008767966	-0.2931174608
H	1.692968011	-0.1571565214	0.7561753418
C	2.4848288282	-0.6902197718	-1.2564738685
C	0.4410135859	0.6914182095	-0.7271115575
H	0.5079274881	1.0378808126	-1.7572590674
C	-0.1720695995	1.6527521895	0.2647807073
C	-3.188677562	-0.6207057795	0.4125095056
H	-1.2185039869	-2.0490737495	1.6231073207
C	-3.0782714705	0.0078863611	1.8206013167
C	-4.0292310024	-1.9173151965	0.5128431793
C	-3.9446916805	0.3728321499	-0.4879971
H	-4.9228948762	0.5991049372	-0.0511800727

H	-4.1145672298	-0.0357739459	-1.489094805
H	-3.4027171511	1.3187180254	-0.5917170598
H	-4.141396554	-2.3847523514	-0.4707816059
H	-5.0291552073	-1.6990113237	0.905801524
H	-3.5570556946	-2.6476621123	1.1769001335
H	-2.5558283154	-0.6445869428	2.5253800967
H	-4.0784375846	0.1955572807	2.2273704106
H	-2.5460338332	0.9619583215	1.7862823619
H	-0.4472774206	1.0879301071	1.1626959345
H	-1.103175275	2.069812215	-0.1339709257
C	0.7763518689	2.7984855201	0.6763433441
H	0.2526788925	3.4463977436	1.393440397
C	1.2957958007	3.6541328178	-0.4897479171
H	1.634443861	2.3707873349	1.2104271873
H	1.9095388808	3.0287815229	-1.1507107608
H	1.9679711874	4.4231794265	-0.0885411123
C	0.1894578854	4.3275499407	-1.3090217547
H	-0.4604906293	4.9356883176	-0.6688443527
H	-0.443839716	3.5909000682	-1.814765207
H	0.6085737398	4.9837488647	-2.0787174992
C	3.4656657047	-1.7642762141	-0.7551593855
H	3.0825926011	0.1788698918	-1.5732083843
H	1.9957100399	-1.0501373337	-2.174208792
H	2.9353439729	-2.7026689743	-0.5559061993
C	4.292762894	-1.3680272057	0.4897584855
H	4.1516163881	-1.9806854202	-1.5832072967
C	3.7075159901	-1.8393316425	1.827733677
H	4.4241296601	-0.2775944421	0.5070299037
H	5.3017385125	-1.7878220316	0.3958421292
H	2.7127776173	-1.4263467599	2.0148173716
H	4.3511614783	-1.5484722049	2.6647816619
H	3.6142187762	-2.9314514677	1.8447922229
H	3.6142187762	-2.9314514677	1.8447922229

TS endo 0634

E(RB3LYP) = -706.409941486 A.U.

First frequency = -539.4504 cm⁻¹

H	-0.7690305572	0.4638932809	-1.8248646952
C	-0.5646386005	-0.3056647757	-1.0901015595
H	0.3195216412	-0.8874040706	-1.3044091112
C	-1.5798542912	-0.8302638564	-0.2982781101
C	-1.2176939203	-1.7437469409	0.7161595566
C	0.0866297939	-2.1919238871	0.8912262624
H	0.314821025	-2.8246616059	1.745243593
H	0.6970525023	-2.4001202647	0.0194846595
C	1.3866138216	-0.4889703233	1.220476575
H	1.133981798	-0.5241003192	2.2787944523
C	2.7431319261	-1.1059885064	0.9076090507
C	0.8696885454	0.6083426947	0.5244588036
H	1.4281941647	1.010003696	-0.3144363216
C	-0.054813966	1.5481951473	1.2603686709
C	-3.051791674	-0.3691813884	-0.3987853493
H	-1.9429514673	-1.9658020379	1.4957227216
C	-3.2956693637	0.5651280987	-1.5984853523
C	-3.5216911951	0.3575368287	0.8813147614
C	-3.9243803996	-1.6317088745	-0.6050462845
H	-4.9788901731	-1.3532340569	-0.714358277
H	-3.8464531076	-2.3217085921	0.2399211082
H	-3.6177886874	-2.1726633637	-1.5061006463
H	-3.3626952786	-0.2497690259	1.7769452657
H	-4.5926215832	0.5824667768	0.8181998676
H	-2.9897925148	1.3031111058	1.01551736
H	-4.3612464657	0.8082253647	-1.6672558579
H	-2.9973827017	0.0944474841	-2.540574092
H	-2.7530272345	1.5100082306	-1.5015129692
H	0.4708019623	1.9385198753	2.1465096406
H	-0.8884412609	0.9540496437	1.6580352861
C	-0.5862996844	2.7364923689	0.4526248119
H	-1.0930372693	2.3677903883	-0.4458738523
C	0.4895732989	3.7503521405	0.0419460458
H	-1.350919364	3.2574797147	1.044863564
H	1.2592410493	3.2525283418	-0.5614062997
H	1.0010149257	4.117779147	0.942131799
C	-0.0838999287	4.9316033187	-0.7459427946
H	0.6961688411	5.6457634611	-1.0292095946

H	-0.833515185	5.4717018106	-0.1561712023
H	-0.5736185755	4.5897152597	-1.6651260091
C	3.1524426892	-1.1401789287	-0.5716420371
H	2.774504639	-2.1226663207	1.3171151685
H	3.5108558038	-0.5438555074	1.4621243618
H	2.4089224917	-1.6991538567	-1.1556289747
C	4.5375377565	-1.7614264737	-0.8147282508
H	3.1508309021	-0.1199185199	-0.9731343247
C	4.6197994968	-3.2584643944	-0.4941142774
H	5.2857939053	-1.2167382657	-0.2226665034
H	4.8108464668	-1.6075171079	-1.8662000492
H	4.4479239698	-3.4596366389	0.5679432497
H	5.6046426398	-3.6631616711	-0.7488185792
H	3.8703993861	-3.8215635237	-1.0627612306
H	3.8703993861	-3.8215635237	-1.0627612306

TS endo 0636

E(RB3LYP) = -706.408436182 A.U.

First frequency = -504.2076 cm^{-1}

H	-1.5937503813	-0.1971353288	-2.1583205145
C	-1.1221721202	-0.6798587307	-1.3075943203
H	-0.2032518459	-1.1962137978	-1.555432485
C	-1.8838667058	-1.0724224166	-0.2116027838
C	-1.198470953	-1.594390576	0.9092941579
C	0.1673729564	-1.823801865	0.9164667038
H	0.6456004596	-2.1297788372	1.8419428474
H	0.6731542617	-2.1590023299	0.0185552127
C	1.1877540212	0.1476580773	0.3883864727
H	1.1967066562	0.3555593055	1.455333657
C	2.4909893316	-0.3479108487	-0.2055768436
C	0.2892315473	0.8659414019	-0.3974497141
H	0.5741836724	1.0701246091	-1.4262820549
C	-0.6746726258	1.8286884835	0.2536237692
C	-3.4134217337	-0.8558941279	-0.2005525323
H	-1.7214441052	-1.6597716988	1.8577949459
C	-4.0339095658	-1.0714741085	1.1928701926
C	-4.0262339047	-1.8981270973	-1.168708672

C	-3.8153632257	0.5563127446	-0.6777360268
H	-4.9064104379	0.6281592245	-0.7478913226
H	-3.4100476382	0.7939754172	-1.6649312499
H	-3.4724476419	1.3223069696	0.0218927118
H	-3.6549264559	-1.751194632	-2.1876370614
H	-5.1195169751	-1.8159435011	-1.1873372635
H	-3.7643834183	-2.9157900185	-0.8610913923
H	-5.116469293	-0.9151233353	1.1435285335
H	-3.6295077213	-0.3678887212	1.9282695953
H	-3.8663780991	-2.0880985163	1.561834153
H	-1.2660989356	1.2629151948	0.9869663734
H	-1.3823116756	2.2056189517	-0.4927644934
C	-0.0381356587	3.0301809805	0.9870143578
H	-0.8454015409	3.5472972052	1.5229784079
C	0.68985662	4.0576681024	0.1031793842
H	0.653062264	2.66392046	1.7577502784
H	0.8082557082	4.9832805533	0.6814815516
H	0.0484080386	4.3174294419	-0.7506220127
C	2.0729477702	3.6274527742	-0.4022420661
H	2.7166364282	3.3278927119	0.4329606954
H	2.570048204	4.4488834844	-0.9295081275
H	2.0156484885	2.7784996261	-1.0873351027
C	3.3965738465	-1.1080703597	0.7717523265
H	3.0530321639	0.5176424254	-0.5900715795
H	2.2755668061	-0.9678144311	-1.0878164057
H	3.531003098	-0.4911874865	1.670617004
C	4.7759374328	-1.4631831786	0.1968060942
H	2.900782063	-2.0281374196	1.1039952267
C	4.7259415275	-2.4496536927	-0.9758703973
H	5.3921680484	-1.890919836	0.9977095131
H	5.2843168094	-0.5422586172	-0.1204548191
H	4.2016893447	-2.0285188107	-1.8397056678
H	4.2049721194	-3.3710717222	-0.6899784392
H	5.7329676815	-2.7246223297	-1.3058383793
H	5.7329676815	-2.7246223297	-1.3058383793

TS endo 0646

E(RB3LYP) = -706.408430420 A.U.

First frequency = -555.0636 cm⁻¹

H	-0.7720210679	-0.6999340772	-2.1467499953
C	-0.534154825	-0.9441424886	-1.1176270823
H	0.2360230534	-1.6971290017	-1.0212282527
C	-1.4896835046	-0.7989004906	-0.1118853851
C	-1.0717113076	-1.0235730324	1.2172229481
C	0.2184050243	-1.4140641475	1.5399542118
H	0.5215128087	-1.4451726505	2.5831129538
H	0.748497275	-2.1123627039	0.903860709
C	1.6230495797	0.0774998408	0.6223206423
H	1.4685890973	0.7127978068	1.487514921
C	2.908446944	-0.7348370117	0.6994340749
C	1.0742493782	0.5102427851	-0.59085302
H	1.5775747747	0.1878374461	-1.498846043
C	0.3889337246	1.8636055167	-0.7349856253
C	-2.9302253022	-0.3147906032	-0.3855932498
H	-1.7201679008	-0.6931129217	2.0254695932
C	-3.8784885874	-1.473781505	0.009696258
C	-3.1681182337	0.0149590196	-1.8702796795
C	-3.3082000409	0.9357744738	0.4386174465
H	-2.7186152373	1.8011859649	0.1295219568
H	-3.1558989552	0.7888863471	1.5112379061
H	-4.3657907897	1.180356708	0.2883605173
H	-2.5230460587	0.8312265837	-2.212686806
H	-4.2060352161	0.3309700743	-2.0180017978
H	-2.9908224886	-0.8530406048	-2.5128296552
H	-3.7830817261	-1.7193407418	1.0717450027
H	-3.6478526008	-2.3775169195	-0.5635290836
H	-4.9226648316	-1.2008601014	-0.1834316741
H	-0.4778541179	1.7778954631	-1.4011368908
H	1.0893554891	2.5374143433	-1.2537077774
C	-0.054079608	2.5431351276	0.5652670282
H	-0.6882763725	1.858505789	1.1396083854
C	-0.7989435923	3.859861778	0.320061775
H	0.8219049456	2.7488625755	1.1941405665
H	-1.645966584	3.6832197979	-0.3568226494
H	-0.1350050633	4.5573142891	-0.2087982983

C	-1.305617217	4.5040949421	1.6130982373
H	-2.0058460358	3.8389917808	2.1313829829
H	-1.823544658	5.4488458346	1.4184256881
H	-0.4780152299	4.7118360975	2.3009956824
C	3.1741523801	-1.729285135	-0.4382161861
H	2.9407184632	-1.277585498	1.6535455487
H	3.7529222943	-0.0286920278	0.7403586735
H	2.3404157884	-2.4387615345	-0.525163783
C	4.4752395666	-2.516379796	-0.2422513031
H	3.2216424039	-1.1992958067	-1.3981442319
C	4.7540904137	-3.5009596783	-1.3812518845
H	4.429231781	-3.0591347387	0.7115782711
H	5.3126110154	-1.8113287081	-0.1502145004
H	4.8372637755	-2.9793468668	-2.3416185988
H	3.9453000634	-4.2348312545	-1.4743218593
H	5.686471152	-4.0512007713	-1.2186577516
H	5.686471152	-4.0512007713	-1.2186577516

TS endo 0650

E(RB3LYP) = -706.408362607 A.U.

First frequency = -549.2043 cm^{-1}

H	-1.4677332025	-0.918576556	-2.1832153553
C	-1.0175326471	-1.1003121355	-1.213506389
H	-0.3039803341	-1.917317425	-1.2224242979
C	-1.7283966109	-0.8202711665	-0.0435986021
C	-1.0496014911	-0.9915398273	1.1814454292
C	0.238758425	-1.4889505202	1.2685703584
H	0.7455670839	-1.4785972245	2.2288421036
H	0.5767211258	-2.2620149682	0.5897738274
C	1.5392779555	-0.2223830694	-0.1784732506
H	1.7493371123	0.4193295367	0.6696331344
C	2.6067059001	-1.2452950872	-0.5176884744
C	0.687985827	0.2452843094	-1.1854400054
H	0.9082085281	-0.1183366676	-2.1888113407
C	0.1010131865	1.6504644749	-1.1711957966
C	-3.1582336692	-0.2392850354	-0.0461548118
H	-1.4857512334	-0.5552237511	2.0774862009

C	-3.6978546433	-0.0088597907	-1.4693672793
C	-3.2541843445	1.1013038654	0.7155968752
C	-4.0727768661	-1.2744949609	0.654130932
H	-5.1120347956	-0.9253598104	0.6655839462
H	-3.7609370867	-1.4438281446	1.6891596042
H	-4.0396442561	-2.237330202	0.1341400535
H	-4.2973736848	1.4332882448	0.765401166
H	-2.679085662	1.879865613	0.2102876793
H	-2.8863443472	1.0230592414	1.742185797
H	-4.7206538261	0.37882618	-1.4195429371
H	-3.7223543242	-0.936717873	-2.0493353469
H	-3.0951754081	0.7218171602	-2.0193163531
H	-0.9215492772	1.6326128742	-1.5674983811
H	0.6793663976	2.2609399097	-1.8823126456
C	0.0945255617	2.3676250503	0.1834599902
H	-0.4362042978	1.7545168929	0.9202120715
C	-0.536905443	3.7622556351	0.1121803342
H	1.1229839251	2.4700406319	0.5530409794
H	-1.5466336505	3.6897890752	-0.3139288212
H	0.0385977143	4.3834442306	-0.5878342964
C	-0.6091038804	4.4502736234	1.4778754594
H	-1.2178426313	3.8657080582	2.1771563439
H	-1.0506174256	5.4494746456	1.4045953615
H	0.3885237396	4.5569143025	1.9191117773
C	3.5150540989	-1.6304193478	0.6563701845
H	3.2254778891	-0.8447179693	-1.3325307639
H	2.139660707	-2.1529050197	-0.9340510995
H	4.0038611608	-0.722524409	1.0381254418
C	4.5869061071	-2.6749146107	0.3089604528
H	2.901847868	-2.0138370887	1.4790774163
C	5.6300307524	-2.1966199983	-0.7078390366
H	4.0953950228	-3.5819583084	-0.0694334935
H	5.0999242834	-2.9712263837	1.2326805285
H	5.1811825525	-1.9806948208	-1.6825540382
H	6.4051118497	-2.95383066	-0.8648103998
H	6.12326505	-1.2810094861	-0.3608968157
H	6.12326505	-1.2810094861	-0.3608968157

TS endo 0657

E(RB3LYP) = -706.408823415 A.U.

First frequency = -537.5043 cm⁻¹

H	-1.6929308106	0.3686368609	-1.964068951
C	-1.1715310771	-0.3389830871	-1.3304313233
H	-0.3982281284	-0.8940494052	-1.8468771499
C	-1.7823277423	-0.8708102562	-0.1994970766
C	-1.0008316077	-1.698915647	0.6369847654
C	0.2966541237	-2.0772464719	0.3217003602
H	0.8703481718	-2.6408473616	1.0519303233
H	0.5568876425	-2.2928049454	-0.7083931846
C	1.5049425637	-0.2338972914	-0.0277160677
H	1.7696372309	-0.2546406044	1.0256518637
C	2.5543125751	-0.7407221369	-1.002182578
C	0.6207590396	0.769956833	-0.4270802082
H	0.7396859537	1.1877303956	-1.4227612095
C	-0.0224493803	1.6427712077	0.6246670647
C	-3.2201666745	-0.5076023228	0.2330843831
H	-1.3664050279	-1.9167452592	1.6377728828
C	-3.268723481	0.1407354609	1.6351312136
C	-4.0337820576	-1.8247885218	0.2674375749
C	-3.9091041403	0.4504980103	-0.755457214
H	-3.3971213111	1.4158191213	-0.8087730928
H	-4.9373630048	0.6407351373	-0.4304425921
H	-3.9522352845	0.0275256528	-1.7640060076
H	-5.0749862341	-1.6263800851	0.5473972933
H	-3.6185746351	-2.5332049925	0.9904599136
H	-4.0290545017	-2.3094375816	-0.7142446507
H	-2.7666486402	1.1119067984	1.6392510546
H	-2.7971868756	-0.486049995	2.3968614485
H	-4.3091591618	0.3018627428	1.9393624673
H	0.7594145647	2.0441220215	1.2876563157
H	-0.6281859885	0.9886530738	1.2652853981
C	-0.8666970821	2.8136380226	0.0916846477
H	-1.3707655846	2.5033456625	-0.8318720677
C	-0.0767613519	4.1079262374	-0.1680371356
H	-1.6635177058	3.043109945	0.8100028823

H	0.3590320912	4.4524062197	0.7799132207
H	-0.7799399885	4.8907010328	-0.4808685506
C	1.0350493181	3.9852953688	-1.2155173732
H	1.8070458523	3.2758769197	-0.9014664039
H	1.5220944241	4.9508579821	-1.3875771332
H	0.6362701583	3.6372393402	-2.1757212986
C	3.4801962123	-1.8541090315	-0.4881080661
H	3.1827984973	0.1083761197	-1.310977156
H	2.055063952	-1.0787184815	-1.9224422568
H	2.8939868659	-2.7387277812	-0.2120022513
C	4.3601812791	-1.4421781953	0.6992135114
H	4.1322193046	-2.1704890061	-1.31335152
C	5.3184640047	-2.5540529462	1.1362253659
H	3.7297459644	-1.1549300569	1.5498949212
H	4.932724096	-0.5443858593	0.428576311
H	5.9898021592	-2.840288496	0.3184654088
H	4.7671061518	-3.4520001599	1.4382502433
H	5.9379507224	-2.242625276	1.9835077079
H	5.9379507224	-2.242625276	1.9835077079

TS endo 0658

E(RB3LYP) = -706.409671367 A.U.

First frequency = -532.8932 cm^{-1}

H	-0.7004576189	0.3924775852	-2.020566138
C	-0.4922132255	-0.3371084278	-1.2475409877
H	0.3308661094	-0.9972706096	-1.4809590362
C	-1.4755671877	-0.7335723835	-0.3484887992
C	-1.0998077463	-1.6018149161	0.7010030856
C	0.1854935537	-2.1035955929	0.8382457182
H	0.4348085047	-2.6829932767	1.7234410996
H	0.7523356227	-2.381527617	-0.0427193459
C	1.5655363302	-0.4070530346	0.9823412316
H	1.3068935946	-0.2912352456	2.0332838854
C	2.8763729364	-1.1510773935	0.7595751637
C	1.1257286694	0.6171678423	0.1396664163
H	1.6959769412	0.8210940907	-0.7626799179
C	0.3689942422	1.7933567948	0.7175371842

C	-2.923975985	-0.1982806021	-0.3870326654
H	-1.7878167367	-1.7360194271	1.5319370691
C	-3.850792863	-1.409507473	-0.6553085384
C	-3.146438521	0.8280860961	-1.5119684096
C	-3.3416892722	0.4582106672	0.947701843
H	-2.7272955262	1.334534145	1.165922901
H	-3.2578148787	-0.2310806588	1.7920730434
H	-4.3860350908	0.7865364438	0.8959926493
H	-2.917822669	0.4067880311	-2.4958556405
H	-2.5334370975	1.7229975005	-1.3715994832
H	-4.194499082	1.145150065	-1.5222937206
H	-3.5942730804	-1.8921852921	-1.6039423291
H	-4.8980770212	-1.0889965942	-0.7050124739
H	-3.7638147157	-2.1609845643	0.1352017215
H	0.9518074953	2.210912542	1.5542228366
H	-0.5653097778	1.4311950236	1.1640030325
C	0.1044266801	2.9187298931	-0.2892961111
H	1.0448959081	3.1448982817	-0.8104455648
C	-0.4327573256	4.2170071128	0.3307414674
H	-0.5891607114	2.5648795969	-1.0608267076
H	-0.4978404288	4.9805920304	-0.4549214703
H	0.2961420116	4.5941424062	1.061327211
C	-1.8009601807	4.0776880943	1.0065848023
H	-2.1621617994	5.0443826803	1.3726885968
H	-1.7603655561	3.397547836	1.8633248571
H	-2.5483003999	3.6853954349	0.3076337045
C	3.2894687122	-1.3772884808	-0.7016666235
H	2.8352827505	-2.1149028409	1.2800515255
H	3.6796211833	-0.5854155088	1.2572983961
H	2.4855916096	-1.8913083193	-1.2460622953
C	4.5881106826	-2.1851442951	-0.8582014149
H	3.4179216996	-0.406946779	-1.195638225
C	4.472228541	-3.6510322834	-0.4240423761
H	5.3890438865	-1.6943425834	-0.28833849
H	4.8982427609	-2.1500866018	-1.9101178925
H	3.6721663457	-4.1592515911	-0.975006206
H	4.2492368108	-3.7458719841	0.6433049232
H	5.4040446671	-4.1937194384	-0.6132899086

H 5.4040446671 -4.1937194384 -0.6132899086

TS endo 0661

E(RB3LYP) = -706.407789068 A.U.

First frequency = -516.6432 cm^{-1}

H -0.8315453606 -0.6713523718 -1.9664028794
C -0.714823592 -1.0874672492 -0.9702349252
H 0.0185838707 -1.8795626439 -0.9114234289
C -1.7585128355 -1.0218490067 -0.0518943603
C -1.5019569046 -1.4699373817 1.2630626616
C -0.282766514 -2.0091223023 1.6414470519
H -0.1042867289 -2.2382092465 2.688582458
H 0.2838771442 -2.622680902 0.9502413
C 1.2929952259 -0.4819106366 1.2244271536
H 1.0034443974 0.0263756145 2.1420588433
C 2.5270161964 -1.3614777998 1.3800726761
C 0.9297100993 0.1621975449 0.0395944079
H 1.5237442841 -0.0105457385 -0.8519850394
C 0.2217886734 1.4939651925 0.1124794556
C -3.1168018276 -0.4003740642 -0.4482293358
H -2.2023700558 -1.2135351652 2.0508922669
C -2.9613705187 0.948834386 -1.182960968
C -4.0394213737 -0.1670602923 0.7631081374
C -3.8142329767 -1.4033917976 -1.4004154477
H -3.2204824 -1.5606081265 -2.3061559167
H -4.8025889749 -1.0338057507 -1.6985489457
H -3.9444416599 -2.3753419621 -0.9134190068
H -4.9886156177 0.2629449994 0.427012875
H -3.5945121909 0.5295684262 1.4814958295
H -4.2697282467 -1.100048361 1.2867733431
H -2.3109474297 0.8737273785 -2.0585814294
H -2.5508504515 1.7150748328 -0.5206696247
H -3.9399052103 1.295749466 -1.5330491071
H -0.6081540927 1.4121176432 0.8285408012
H -0.224026192 1.7303888655 -0.8565929578
C 1.1456751734 2.6466121243 0.5486655953
H 1.6272759712 2.3758276736 1.4966605608

C	0.4211446618	3.9917207103	0.7140800974
H	1.9572743167	2.7561773427	-0.1849106132
H	1.1294509475	4.7272705899	1.1165147796
H	-0.3678823196	3.8822279545	1.4711138676
C	-0.1893200429	4.5414603666	-0.5806361452
H	-0.9834565816	3.8926554856	-0.9638755689
H	0.5713929934	4.6314525442	-1.3651366928
H	-0.6243536237	5.5337935931	-0.4228945849
C	3.0771913142	-2.0083901033	0.093740048
H	2.3226479146	-2.1437298119	2.1208253386
H	3.3234567622	-0.747653785	1.8283847791
H	3.5751324167	-2.9525222396	0.3482247423
C	4.079344705	-1.1291549995	-0.6695429718
H	2.2481395093	-2.2833497495	-0.5720922791
C	4.5126317366	-1.742646943	-2.0031557973
H	4.9592314558	-0.9681980961	-0.0321274695
H	3.6503421304	-0.1349856305	-0.840582206
H	5.2485294658	-1.1150798451	-2.5161917243
H	3.6552613308	-1.8686355131	-2.6745611109
H	4.9619360017	-2.73155732	-1.8554075597
H	4.9619360017	-2.73155732	-1.8554075597

TS endo 0662

E(RB3LYP) = -706.409508801 A.U.

First frequency = -533.5581 cm^{-1}

H	-1.6187528686	0.3311014729	-2.0295141141
C	-1.1537905666	-0.3990245869	-1.3775396785
H	-0.4084043268	-1.0093453031	-1.8713501041
C	-1.8097195761	-0.8676123342	-0.2447057129
C	-1.094652136	-1.7295483753	0.617942695
C	0.1715230988	-2.2108572984	0.3204293994
H	0.6991515638	-2.802339749	1.0630851664
H	0.4191577826	-2.4620136999	-0.7047399082
C	1.5191887256	-0.4741586437	-0.0309398197
H	1.7529495272	-0.4873740337	1.0299360878
C	2.5577242162	-1.0806295956	-0.9579768031
C	0.7303936769	0.5880839823	-0.474632443

H	0.9061525037	0.9633270364	-1.4795563056
C	0.1559905599	1.5429027296	0.5421004097
C	-3.2239155917	-0.4013473954	0.1681034347
H	-1.4803810408	-1.8929827941	1.6217738486
C	-3.89444912	0.470666454	-0.9095509275
C	-3.2121702928	0.3914688844	1.4945399767
C	-4.0967183655	-1.6673375793	0.3530336207
H	-5.1233124058	-1.3881296196	0.6169831239
H	-3.7108766915	-2.3134386014	1.1466549579
H	-4.1280922066	-2.2556523332	-0.5696898489
H	-4.2372814662	0.6212164872	1.8072144924
H	-2.6769028766	1.3381987368	1.3853049511
H	-2.7386124692	-0.1730540758	2.3028273248
H	-3.3628924617	1.4136871475	-1.0672168112
H	-4.9149718015	0.7206800045	-0.6009853016
H	-3.9526615153	-0.0526316701	-1.8691419658
H	0.9749744067	1.9339314834	1.1628687692
H	-0.4712606089	0.9631949772	1.232819321
C	-0.646326157	2.72005145	-0.0259676058
H	-1.5123374798	2.3307380341	-0.5711007506
C	0.1382807925	3.6617962968	-0.955796766
H	-1.0458039145	3.3067302238	0.8124644447
H	-0.5409771584	4.4528950704	-1.2981272252
H	0.4435245449	3.1210027676	-1.8607891062
C	1.371371195	4.299751427	-0.3072370416
H	1.8407012	5.0259028118	-0.9789119148
H	2.1271652866	3.5490126761	-0.0549362074
H	1.1033943764	4.8242262184	0.6175006457
C	3.3339164695	-2.296298821	-0.4202330786
H	3.2811867932	-0.2967672234	-1.2228196608
H	2.0770453517	-1.3564275132	-1.9080821382
H	2.6685984809	-3.1637642716	-0.3481575607
C	4.0189562346	-2.0844324556	0.9403990443
H	4.0990542415	-2.5620481192	-1.1619510979
C	4.9734360206	-0.8862320777	0.9796509508
H	4.5711937745	-2.9979542122	1.1945240928
H	3.2587306812	-1.969724612	1.7235248834
H	4.4375865986	0.058314772	0.8401974686

H	5.7295898827	-0.958212491	0.1890671475
H	5.4979023114	-0.8289622353	1.9388801282
H	5.4979023114	-0.8289622353	1.9388801282

TS endo 0663

E(RB3LYP) = -706.409603400 A.U.

First frequency = -530.8905 cm⁻¹

H	-0.877958887	0.0739576938	-2.0138898413
C	-0.6731156082	-0.568101482	-1.1659821617
H	0.093497833	-1.3063541695	-1.3526487422
C	-1.6265404063	-0.7820154981	-0.1776559295
C	-1.2476721111	-1.5399453518	0.953221211
C	0.0100482617	-2.1073521492	1.0907994855
H	0.2712620347	-2.5922010942	2.0278493062
H	0.5089949288	-2.5269716247	0.2247492984
C	1.4949897788	-0.5051150448	0.9651269301
H	1.2952297546	-0.2400172288	2.0018138356
C	2.7488932707	-1.3521024543	0.7871687547
C	1.0812490268	0.4334153588	0.0159245319
H	1.6170813641	0.4793570601	-0.9284202647
C	0.433638038	1.7242476412	0.4676956193
C	-3.0378006645	-0.1550491136	-0.2126811071
H	-1.8953289423	-1.5244535665	1.8262782613
C	-3.2587620843	0.737172374	-1.4469702647
C	-3.3344600281	0.6898383596	1.0463516102
C	-4.0539531358	-1.3216946906	-0.2779578044
H	-3.9696923729	-1.9733684227	0.5969249866
H	-3.883914016	-1.935440035	-1.1685111067
H	-5.0797705198	-0.9367311541	-0.3166690698
H	-4.3575601465	1.0807009377	1.0058656559
H	-2.6549172478	1.5419474851	1.1190947061
H	-3.24387295	0.1068136764	1.9666727761
H	-4.2833635898	1.1234994738	-1.446400835
H	-3.1139983858	0.1822491171	-2.3791019063
H	-2.5829394177	1.5971761256	-1.4516059587
H	1.0858967384	2.2026463954	1.2159300126
H	-0.496887045	1.4890327064	0.998910175

C	0.1893599152	2.7285512554	-0.664497409
H	1.113470745	2.8193052302	-1.2518605391
C	-0.2291568219	4.1298779722	-0.1958432395
H	-0.5658437354	2.330267505	-1.3518756927
H	-0.2861710883	4.7900966123	-1.0707305659
H	0.559991896	4.5443513646	0.4466032901
C	-1.5660834038	4.1746829837	0.5518153806
H	-1.524232097	3.6082483053	1.487550187
H	-2.372742806	3.749975733	-0.0563431315
H	-1.8447602383	5.2031977415	0.803783171
C	3.081165752	-1.7753234606	-0.6508664363
H	2.6785298788	-2.253827767	1.4105556806
H	3.5952129969	-0.7813224884	1.1951616648
H	2.1997540526	-2.2404663268	-1.110128386
C	4.2604259775	-2.7559634447	-0.7491487713
H	3.3059326042	-0.8876476012	-1.2562800418
C	5.5987582035	-2.1764157844	-0.2766128418
H	4.3601269561	-3.0812364337	-1.7924186496
H	4.0271032554	-3.659257288	-0.1689960479
H	5.8446684032	-1.2602370777	-0.8263371062
H	6.4150421154	-2.8888344441	-0.4338700961
H	5.5810515412	-1.9276839217	0.7891546397
H	5.5810515412	-1.9276839217	0.7891546397

TS endo 0665

E(RB3LYP) = -706.407113061 A.U.

First frequency = -552.2517 cm⁻¹

H	-1.8327827842	-1.3246141993	-2.0108438437
C	-1.2635641515	-1.3246635188	-1.0878178383
H	-0.4538385696	-2.0463794007	-1.0864166138
C	-1.873135872	-0.9673892975	0.1170674633
C	-1.0507388203	-0.8940713369	1.2604865125
C	0.2932557615	-1.2263650485	1.2447959272
H	0.8965224385	-1.0310174962	2.1263855284
H	0.6491900185	-2.0444618449	0.6304851783
C	1.2419046401	-0.0153417149	-0.4652931709
H	1.4466671979	0.7463350856	0.2773321047

C	2.4044247412	-0.9266916076	-0.8107354998
C	0.2442003511	0.2190464292	-1.4184466798
H	0.4133696651	-0.2410176228	-2.39148085
C	-0.5451956063	1.5230603671	-1.4951353622
C	-3.3499217188	-0.5304524385	0.2183640108
H	-1.4382438149	-0.390253471	2.1432888389
C	-3.5001289962	0.9009194461	0.781488383
C	-4.0581051566	-1.5185375632	1.1775499208
C	-4.0738293105	-0.5824513338	-1.139215494
H	-3.6315688553	0.1086677524	-1.8646144642
H	-5.1229802003	-0.2965416063	-1.0109094427
H	-4.0531430008	-1.5881713488	-1.5706883142
H	-3.9818391728	-2.544893257	0.8042141687
H	-5.1205765284	-1.2662565926	1.2749571529
H	-3.6119962278	-1.4933308193	2.1762595733
H	-3.0667864046	1.6392456144	0.1029730643
H	-3.0139545439	1.015579764	1.7539120703
H	-4.5604828882	1.1450924304	0.912597713
H	-1.6008781684	1.2977927374	-1.6754004576
H	-0.2075010051	2.0648191471	-2.3919184726
C	-0.4286192022	2.4708038792	-0.2872542884
H	-1.3118335802	3.1217681862	-0.2587575094
C	0.817999062	3.3675250897	-0.3112081251
H	-0.4611301326	1.8895188953	0.6422330522
H	0.7603438163	4.0256104913	-1.1889564361
H	1.7172610481	2.7573999842	-0.4550423171
C	0.9638213085	4.2107043239	0.9580922098
H	1.8405674126	4.864884409	0.911139771
H	1.0703150186	3.5722196807	1.8428493368
H	0.0826163822	4.8436184082	1.1150819336
C	3.4620860639	-1.066278409	0.2892482313
H	2.8981372861	-0.5433701624	-1.7166051373
H	2.0292225575	-1.9238278	-1.0918772376
H	3.8126870995	-0.0644393452	0.5759806051
C	4.6619935847	-1.9207067116	-0.1331812538
H	3.0127801696	-1.4991765004	1.1908175227
C	5.7174529029	-2.0534733141	0.9682716709
H	5.1195530979	-1.4849615134	-1.0318351694

H	4.3083946813	-2.918749371	-0.4264292001
H	6.1089280517	-1.0717554869	1.2586302933
H	6.5637994179	-2.667522604	0.6438372444
H	5.2932674998	-2.5171905649	1.866247653
H	5.2932674998	-2.5171905649	1.866247653

TS endo 0671

E(RB3LYP) = -706.407096773 A.U.

First frequency = -545.5464 cm^{-1}

H	-1.3364329797	-0.95849788	-2.1476483126
C	-1.1178456348	-1.3175664261	-1.1482459298
H	-0.5811213304	-2.2586215004	-1.1392725132
C	-1.9506838958	-0.9867788335	-0.0777651191
C	-1.5436151517	-1.3973673114	1.2092456821
C	-0.3982970713	-2.1468861658	1.4224336729
H	-0.0565060081	-2.329875249	2.4376957735
H	-0.1152370853	-2.9156357365	0.7135200366
C	1.3191227131	-1.0438315756	0.4548918538
H	1.441433433	-0.4809076604	1.3739719872
C	2.2709368814	-2.2113278999	0.2881233562
C	0.8146902593	-0.3733824918	-0.6691104706
H	1.1572781137	-0.7474361859	-1.6322747318
C	0.521047108	1.1218818946	-0.6730050838
C	-3.2112197482	-0.1095816011	-0.23346811
H	-2.0335094978	-0.9545560659	2.0735394295
C	-3.4415839125	0.33730826	-1.688518111
C	-3.1605260187	1.1591168834	0.6457975966
C	-4.4222612434	-0.969906431	0.2038199357
H	-5.3553364487	-0.4044684493	0.0959602027
H	-4.3330917407	-1.2795432044	1.249455793
H	-4.4968799683	-1.8754677571	-0.4068510301
H	-2.3625671415	1.8291178374	0.3193173606
H	-2.9943452238	0.9263990863	1.701030234
H	-4.1077913592	1.7056900936	0.5752559042
H	-4.3593715248	0.9310066381	-1.7527754703
H	-3.5506985241	-0.517537863	-2.3632161749
H	-2.6200698067	0.960836376	-2.0573037429

H	-0.4022022504	1.327392241	-1.227948241
H	1.3224458851	1.6048890701	-1.2498427295
C	0.426513266	1.7933709473	0.7033822166
H	-0.3280303702	1.2733371807	1.3029749014
C	0.0948132293	3.2921138624	0.6352748955
H	1.3778783603	1.6753003497	1.2387387904
H	-0.095676604	3.6564513595	1.6526373276
H	-0.8417745834	3.4384896978	0.0804096265
C	1.1982968677	4.1450347684	-0.0026472767
H	1.3599716054	3.8831722507	-1.0530694186
H	2.1511817118	4.007274447	0.5217291489
H	0.9470563143	5.2099978636	0.0347188093
C	3.7724601002	-1.8418145675	0.2894239052
H	2.0376488178	-2.7305653367	-0.6526443278
H	2.1205905602	-2.9473699128	1.088068789
H	4.037288469	-1.4283990688	1.2724376796
C	4.232522355	-0.8646521075	-0.812598392
H	4.3328519152	-2.7812843078	0.2000670775
C	4.2216024095	0.6079413831	-0.385624242
H	3.6045538429	-0.9973310343	-1.7030550318
H	5.2513720727	-1.1280158589	-1.1226747648
H	3.2321315925	0.9170878922	-0.0428195315
H	4.5140517255	1.2667501852	-1.2104457786
H	4.9236369083	0.7756910279	0.4393081379
H	4.9236369083	0.7756910279	0.4393081379

TS endo 0672

E(RB3LYP) = -706.408981479 A.U.

First frequency = -518.6171 cm^{-1}

H	-0.9456189573	-0.0298532148	-1.9885228585
C	-0.6620449658	-0.6565806343	-1.1512561753
H	0.238301149	-1.2308169848	-1.3228709546
C	-1.6123444947	-1.1244926791	-0.2491002405
C	-1.1444935009	-1.8335401311	0.8805012831
C	0.1991979339	-2.0718212549	1.1105297332
H	0.511349758	-2.5151747808	2.0522673513
H	0.8760908028	-2.2536871884	0.2863654017

C	1.1928628181	-0.0514940773	1.1469930904
H	0.7350733787	0.1184811987	2.1193261387
C	2.66201142	-0.4498253926	1.252946182
C	0.6464795573	0.6904805087	0.0943815136
H	1.2728614134	0.8723107342	-0.7749399933
C	-0.3680983072	1.7707136927	0.4040629942
C	-3.1149560213	-0.7892315689	-0.359350121
H	-1.8392874702	-2.0248004271	1.6947471802
C	-3.6535550539	-0.0808557265	0.9047633083
C	-3.8723191688	-2.1275798431	-0.5391189737
C	-3.4278617718	0.1074169637	-1.5706481222
H	-3.1268500137	-0.3632271533	-2.5118239737
H	-2.9247130668	1.0770286689	-1.4959396731
H	-4.504985333	0.2968931824	-1.6236908425
H	-3.7162514182	-2.791977149	0.3162253577
H	-3.5269075035	-2.651816691	-1.436008994
H	-4.9496611664	-1.9503018189	-0.6379569687
H	-3.4828007604	-0.6661479553	1.8121693562
H	-4.7342126912	0.0778649121	0.8151245771
H	-3.1826741521	0.8965911617	1.040847352
H	-1.1156422169	1.3596404162	1.0911455623
H	-0.9087261483	2.0617192875	-0.5030336225
C	0.2597423525	3.0215281852	1.0552285569
H	-0.5356651087	3.7578370464	1.2384838675
C	1.3788508436	3.6827147081	0.2352052931
H	0.6601766207	2.7420560876	2.0382497832
H	2.2230185612	2.9864063109	0.1489058593
H	1.7566009253	4.5495399389	0.7920857974
C	0.9447766907	4.1308906309	-1.1644889073
H	0.6603780857	3.2788010614	-1.7909777295
H	1.7518593835	4.6621209366	-1.6794129427
H	0.0809047504	4.8040496106	-1.1131492753
C	3.5308766134	-0.3621253972	-0.0129604945
H	2.7595455168	-1.4498351976	1.6939929123
H	3.1076807258	0.2275895503	1.9964750836
H	3.443548111	0.64664329	-0.4355422914
C	3.249099159	-1.3980082612	-1.1127204218
H	4.5800351159	-0.4670290613	0.2948665382

C	3.5701580602	-2.8413374749	-0.7086380756
H	3.8463533549	-1.137138958	-1.9957166327
H	2.2032534006	-1.3271650708	-1.4318500097
H	4.6218450413	-2.9387389448	-0.4153295511
H	3.3886163011	-3.533601246	-1.537110238
H	2.9621266281	-3.1762475009	0.1373963869
H	2.9621266281	-3.1762475009	0.1373963869

TS endo 0675

E(RB3LYP) = -706.408400113 A.U.

First frequency = -547.0178 cm⁻¹

H	-1.4693546206	0.4289346839	-1.9299933596
C	-1.0657978095	-0.3602193682	-1.3059863312
H	-0.382652558	-1.0164448601	-1.8318440725
C	-1.7752523163	-0.8262552749	-0.2015012307
C	-1.1409772644	-1.776235398	0.6289989367
C	0.0868386241	-2.3459304512	0.3242747439
H	0.5571456435	-2.9982390891	1.054650478
H	0.3280882545	-2.5872510617	-0.7042564052
C	1.5674250181	-0.6930328543	-0.0118021773
H	1.8229254647	-0.8009217377	1.03719717
C	2.5027489229	-1.3487104792	-1.013907704
C	0.8409662101	0.4431846055	-0.3734717453
H	1.0413496736	0.8794351437	-1.3492420267
C	0.3490845491	1.3683974871	0.7137194812
C	-3.1538692441	-0.2675929386	0.2164168927
H	-1.5516620773	-1.9501237952	1.6212436719
C	-3.1042068408	0.4479415322	1.585266313
C	-4.1292493886	-1.4665667744	0.3169176543
C	-3.7306034742	0.7153470587	-0.8191992058
H	-3.8150749058	0.2529838705	-1.807711291
H	-3.1199112809	1.6178669236	-0.9149849917
H	-4.7324610846	1.0319561369	-0.510591883
H	-5.1349532302	-1.1200971878	0.5817131526
H	-3.8106302316	-2.1846096522	1.0779583729
H	-4.1904316664	-1.9985424657	-0.6379658741
H	-2.4927013328	1.3524884722	1.5364347139

H	-2.693723714	-0.1957944237	2.3683639983
H	-4.1135055595	0.7429572793	1.8945216779
H	1.2032120945	1.6614334818	1.3435874751
H	-0.3125140048	0.7904837753	1.3725674977
C	-0.3563893111	2.6386056628	0.2267534786
H	-1.1732502254	2.3624626514	-0.4498007366
C	0.5680218627	3.6369841631	-0.4824370358
H	-0.8242513706	3.1421487662	1.083466978
H	1.0463585782	3.1542675468	-1.3441802571
H	1.3834374945	3.9178450936	0.1980550463
C	-0.170284389	4.8937552042	-0.9517590801
H	-0.9699031913	4.6392199655	-1.6570427381
H	0.504538147	5.5961874051	-1.4516914319
H	-0.6322991519	5.4176870244	-0.1070673777
C	3.388044941	-2.4802074557	-0.4556929959
H	3.1539892405	-0.5812529822	-1.4579329721
H	1.9076855756	-1.7326086505	-1.856086973
H	2.8186237632	-3.0624541043	0.2796922025
C	4.710763245	-2.0119466734	0.1753789398
H	3.6315751662	-3.1751171215	-1.2685603899
C	4.5657651416	-1.0883946375	1.389847428
H	5.3066099672	-1.5019712989	-0.5942024539
H	5.2885886113	-2.8985153834	0.4672516809
H	4.0838582532	-0.1429080056	1.122945445
H	5.5442202993	-0.8513526642	1.8206485941
H	3.9615752171	-1.558657857	2.1745841936
H	3.9615752171	-1.558657857	2.1745841936

TS endo 0680

E(RB3LYP) = -706.405973807 A.U.

First frequency = -545.9239 cm^{-1}

H	-1.9120069923	-1.1198996899	-2.2132140492
C	-1.4377052534	-1.3670001957	-1.270228491
H	-0.7726998238	-2.2198971865	-1.3328618174
C	-2.0542418684	-1.0538864033	-0.0591886351
C	-1.3260000579	-1.3022702539	1.1233016039
C	-0.0630324204	-1.8725159149	1.1125277217

H	0.5075331465	-1.9285776801	2.0360441465
H	0.1723160019	-2.6542232905	0.3999525636
C	1.2013351367	-0.6137266969	-0.2350768656
H	1.4054467151	0.0321502765	0.6090615994
C	2.2776850032	-1.6354523355	-0.5546207073
C	0.4024646275	-0.1091222215	-1.2706960674
H	0.6069822005	-0.514733705	-2.260567049
C	-0.1488236008	1.3155794059	-1.2965539707
C	-3.4128364443	-0.3267113015	0.032231797
H	-1.6764980154	-0.8557749109	2.0510262641
C	-4.3804788795	-1.2488210691	0.8134126335
C	-4.0285401002	-0.0533815108	-1.3519259178
C	-3.301049962	1.022461454	0.7781215856
H	-4.2919123432	1.4788211404	0.8836587497
H	-2.6641198533	1.7233963773	0.2335010462
H	-2.8848309526	0.9050431177	1.7822290077
H	-5.0050344406	0.4279585602	-1.2347059824
H	-4.1784591159	-0.9784693864	-1.917440861
H	-3.4033506236	0.6155274525	-1.9528428185
H	-5.3704144841	-0.785281578	0.897345386
H	-4.0139180406	-1.4469035171	1.8250460722
H	-4.4945114519	-2.2120333559	0.3056436181
H	-1.218326313	1.2955831202	-1.5245815574
H	0.3183732805	1.8365637474	-2.1461485061
C	0.0837172027	2.1600196565	-0.0318732934
H	-0.6462288805	2.9792336356	-0.0053121231
C	1.4937268546	2.7634461985	0.0456331947
H	-0.1223423229	1.5551016483	0.8598513047
H	1.5916695773	3.529061588	-0.7357716991
H	2.2342429395	1.9937621342	-0.1977745237
C	1.8140088015	3.3706297267	1.412887689
H	2.8090538027	3.8274681576	1.4301823734
H	1.7860343783	2.6041869954	2.1961875036
H	1.0861876835	4.1443434315	1.6835242103
C	3.6329473993	-1.0148056505	-0.9863388139
H	1.905312461	-2.282262446	-1.3600634445
H	2.4601358069	-2.2970968	0.3021252479
H	4.0994038367	-1.665924646	-1.7365963521

C	4.6403855126	-0.8233247534	0.1598898306
H	3.4487156672	-0.0554594897	-1.4866003747
C	4.1740378515	0.0909588765	1.297730871
H	5.5748440869	-0.4269366345	-0.2581490632
H	4.8889086062	-1.8101962012	0.574421612
H	4.9570303018	0.2046071385	2.054778174
H	3.2891119734	-0.3117718778	1.8010512998
H	3.9202611542	1.0901424411	0.9292948378
H	3.9202611542	1.0901424411	0.9292948378

TS endo 0683

E(RB3LYP) = -706.407039401 A.U.

First frequency = -551.5531 cm^{-1}

H	-2.0758171197	-1.3334805506	-2.0019017879
C	-1.4633736576	-1.4148171543	-1.1107206112
H	-0.7467213504	-2.2276648371	-1.158408196
C	-1.9617753948	-1.005118159	0.1282279584
C	-1.078530475	-1.048688271	1.2268975342
C	0.2136252847	-1.5378354051	1.13694195
H	0.87963271	-1.4302679585	1.9880548727
H	0.4391900931	-2.3813044026	0.4960399441
C	1.2039111321	-0.4113639705	-0.6062273698
H	1.5097223867	0.3139600081	0.135132568
C	2.2459764287	-1.4378052162	-1.0117625155
C	0.1967449935	-0.0562000477	-1.5105853615
H	0.2687208134	-0.5202364331	-2.493797153
C	-0.4384380861	1.3321148693	-1.5403651231
C	-3.3664022218	-0.392544283	0.3122455252
H	-1.3570449387	-0.5169621759	2.1340983355
C	-3.3090055402	1.0376573236	0.8954960598
C	-4.1405213054	-1.300712511	1.2990275167
C	-4.1607893924	-0.3344371643	-1.0050978687
H	-3.6756830975	0.3088966465	-1.7468490999
H	-5.1589144978	0.0751051654	-0.818158608
H	-4.2860173396	-1.3282898387	-1.4463086775
H	-3.6429116702	-1.3470444264	2.2723224132
H	-4.2122585653	-2.3224609353	0.912393892

H	-5.1567613222	-0.9205881141	1.456294033
H	-2.7669704535	1.07547542	1.8441486228
H	-4.3229294893	1.4101735465	1.0808338889
H	-2.8188859689	1.7269000974	0.2039950174
H	-1.5232308505	1.2356427487	-1.6468941782
H	-0.1000182467	1.833625211	-2.4598750961
C	-0.1263183362	2.2534240156	-0.3471866077
H	-0.9106156351	3.0175676867	-0.2717340574
C	1.2279177654	2.9717388194	-0.4481906854
H	-0.1841074896	1.6799141912	0.5860845345
H	1.2015201147	3.6511727855	-1.310943883
H	2.022312492	2.2477310653	-0.663559781
C	1.5774744841	3.7566372286	0.8186371085
H	0.8040695605	4.4979990674	1.0509151123
H	2.5293291903	4.2878906979	0.7159289815
H	1.6600117153	3.0877065777	1.6833842769
C	3.3572093779	-1.68988818	0.0179465782
H	2.7182424229	-1.1115604929	-1.9508057873
H	1.7495457792	-2.3890465461	-1.257794098
H	2.921881468	-2.0299879665	0.9654014186
C	4.2498993641	-0.4694032962	0.2811836845
H	3.9879936125	-2.5145875058	-0.3397203511
C	5.3770558851	-0.7647119644	1.2748428784
H	3.6442816506	0.3635760053	0.6598573098
H	4.6759657344	-0.1248237284	-0.671133552
H	4.9740346846	-1.081941142	2.243567221
H	6.0037348199	0.1163565551	1.4469845839
H	6.0248637343	-1.5696052277	0.9089415385
H	6.0248637343	-1.5696052277	0.9089415385

TS endo 0687

E(RB3LYP) = -706.407314376 A.U.

First frequency = -546.7027 cm⁻¹

H	-1.3172502705	-0.5942398791	-2.2491084638
C	-0.8796350246	-0.901672462	-1.3057682735
H	-0.1000308457	-1.6469779806	-1.4209320648
C	-1.6394164649	-0.8752862433	-0.1340672761

C	-0.9799710774	-1.1973171278	1.0712851308
C	0.3418622023	-1.603288513	1.123294531
H	0.8238888491	-1.7161381254	2.0897091001
H	0.7570116469	-2.2239963525	0.3389308607
C	1.5692398824	-0.0138140495	-0.0330639508
H	1.6995910241	0.4953748048	0.915061519
C	2.7285356658	-0.8796607987	-0.4870180761
C	0.7145812167	0.5472185693	-0.9880451748
H	0.9923862262	0.3659090333	-2.026012292
C	0.0207451493	1.8873166114	-0.7780298048
C	-3.11033385	-0.4101946932	-0.0957724617
H	-1.4719172969	-0.9508573441	2.0097139369
C	-3.6292547831	0.0170765366	-1.4807209899
C	-3.3305165274	0.7715587718	0.8740192836
C	-3.9576422368	-1.6134814126	0.3862814307
H	-3.6594354775	-1.9323866597	1.3895632954
H	-3.8355844482	-2.469171401	-0.2856358451
H	-5.0211666379	-1.3487383682	0.4163471245
H	-2.8013761481	1.6626006011	0.5302675945
H	-2.9876132517	0.5467779635	1.8874847091
H	-4.3969823776	1.0163026548	0.9352761917
H	-3.0719244932	0.8724406788	-1.8773604389
H	-4.680396618	0.314648871	-1.4068923307
H	-3.5654392616	-0.7986439505	-2.2076527528
H	-0.9917863813	1.8575687531	-1.1993520711
H	0.5662686837	2.630499115	-1.3770987596
C	-0.0621415516	2.3828074418	0.6720424152
H	-0.5425246603	1.6130533354	1.284989758
C	-0.8149725884	3.7135414696	0.8284183299
H	0.9516956867	2.5097109905	1.0739110371
H	-0.9512700893	3.9156757171	1.8983502525
H	-1.8248816537	3.6181546262	0.4075031145
C	-0.1107214986	4.9114901884	0.1799245294
H	-0.6531969243	5.8423078538	0.3750655625
H	-0.0327757689	4.7995721762	-0.9061901207
H	0.9056865274	5.0283880918	0.5739039749
C	3.6124090474	-1.4143747891	0.6470402509
H	3.3643999102	-0.293612135	-1.1688628954

H	2.3470909049	-1.7114469953	-1.0979518246
H	3.9265257837	-0.5661489165	1.2701907698
C	4.8590877008	-2.1709231764	0.1644628739
H	3.0263609253	-2.0718054467	1.3002292612
C	4.5466071978	-3.4707788847	-0.5862907553
H	5.488673953	-2.4025900426	1.0328738296
H	5.4577442222	-1.5111385042	-0.4786224887
H	3.9327322613	-4.1396104356	0.0284854802
H	5.4641023818	-4.0074253575	-0.8487175687
H	3.9999000558	-3.2826278938	-1.5158675315
H	3.9999000558	-3.2826278938	-1.5158675315

TS endo 0690

E(RB3LYP) = -706.408968804 A.U.

First frequency = -539.5195 cm^{-1}

H	-0.4615293029	0.0325709619	-1.8847500274
C	-0.4677574541	-0.6715145558	-1.0615256497
H	0.2474915113	-1.4739030074	-1.170870004
C	-1.5994499033	-0.8470473147	-0.2726257199
C	-1.4900577017	-1.6983075436	0.8484547183
C	-0.3293103692	-2.4052763047	1.1375168437
H	-0.276851003	-2.977682308	2.060218177
H	0.249656405	-2.8323119887	0.3252670802
C	1.315347406	-1.0134261846	1.3771717647
H	1.0038844666	-0.8287508797	2.4039773487
C	2.4921413943	-1.9786648494	1.2753056848
C	1.1116099617	0.0577826131	0.4991891667
H	1.7766362216	0.1818887214	-0.3491102628
C	0.4641504421	1.312489343	1.0352359576
C	-2.91602228	-0.07016789	-0.498036691
H	-2.2688954359	-1.6614041079	1.606649735
C	-2.9025947881	0.7467503049	-1.8034783101
C	-3.2254414703	0.8916387862	0.6701768282
C	-4.0604354803	-1.1074573203	-0.6086555144
H	-4.1692162895	-1.6920888085	0.309177342
H	-3.872211694	-1.8073325895	-1.4291594787
H	-5.0148230704	-0.6034412947	-0.799930982

H	-4.2063843066	1.3597565072	0.5286629256
H	-2.4803454261	1.6890064306	0.7282513374
H	-3.2401561036	0.3731884351	1.6330803894
H	-2.701814421	0.1117185625	-2.6720327467
H	-2.1536363318	1.5439479236	-1.7834640582
H	-3.8779471377	1.2217494612	-1.9527236268
H	1.0761530685	1.6912737451	1.8693292048
H	-0.5019017818	1.0432876994	1.4843860188
C	0.284399929	2.4397188263	0.0179243229
H	1.2484243064	2.6459584385	-0.4690349089
C	-0.2548728145	3.7357881051	0.6323158221
H	-0.389611152	2.1066072918	-0.7782018237
H	0.4468230842	4.0944945669	1.3974878944
H	-1.1944053049	3.5258063422	1.1612049817
C	-0.4905730331	4.8331558741	-0.4090611494
H	0.4371467547	5.0806421076	-0.9377179124
H	-0.8686355342	5.752232345	0.0503060501
H	-1.22091868	4.5100782509	-1.159945024
C	3.0914712571	-2.1937002994	-0.1292554968
H	2.1972202199	-2.9476583458	1.6956794466
H	3.2885107122	-1.6112192649	1.9403792193
H	3.5021875604	-3.2091064203	-0.1952080974
C	4.2071470291	-1.2030251531	-0.4949519037
H	2.2991385682	-2.1478908418	-0.8878396866
C	4.7004494206	-1.3700512618	-1.9342306963
H	5.0436037888	-1.3447608568	0.2026789618
H	3.8611700287	-0.1745569872	-0.3393752386
H	3.8910741435	-1.186761092	-2.6504683786
H	5.0699420586	-2.3871097555	-2.1094200416
H	5.5141156819	-0.6749925454	-2.1653475297
H	5.5141156819	-0.6749925454	-2.1653475297

TS endo 0693

E(RB3LYP) = -706.407117345 A.U.

First frequency = -498.8533 cm^{-1}

H	-2.1048701738	-0.2494554302	-2.0264776527
C	-1.4593165424	-0.7963323446	-1.3457914061

H	-0.7064307398	-1.3928869461	-1.8452248972
C	-1.9077070106	-1.138921251	-0.0745187786
C	-0.984093927	-1.7538228986	0.8028703508
C	0.295214046	-2.1137305839	0.4196633297
H	0.9860687959	-2.492051925	1.1658871819
H	0.4938027727	-2.452724664	-0.5900458248
C	1.3068628649	-0.2039992736	-0.3701922393
H	1.5965935875	-0.0002798041	0.6546811356
C	2.3677219618	-0.7997094568	-1.275683457
C	0.2963108484	0.5895402658	-0.9064876775
H	0.3197911942	0.7740162624	-1.9784762684
C	-0.354740703	1.6486973407	-0.0476564488
C	-3.3406928967	-0.7796053196	0.3771986791
H	-1.2177555149	-1.7949503177	1.8617545238
C	-3.7239736502	0.675687592	0.0330892656
C	-3.5522064399	-0.9714431473	1.8910869716
C	-4.3046646723	-1.7346448096	-0.3698026217
H	-5.3435642368	-1.5504634518	-0.0712341085
H	-4.0649527283	-2.7799457295	-0.1491083125
H	-4.230660238	-1.5965043922	-1.4529125328
H	-2.8861924606	-0.3288024526	2.4766055619
H	-3.3867874558	-2.0085923581	2.1987920949
H	-4.5823398568	-0.711601738	2.1558727265
H	-4.7772959515	0.8504610237	0.2789975603
H	-3.5968873421	0.9001053298	-1.0293649873
H	-3.1230291682	1.3879461341	0.6035439262
H	-0.7217229142	1.1707717337	0.8704251817
H	-1.2313461346	2.0580952484	-0.560723903
C	0.5901594099	2.8059021053	0.3341222815
H	0.0567898679	3.4935411432	1.0056289485
C	1.125100881	3.590973982	-0.8687275368
H	1.4375257216	2.408689078	0.9090965624
H	0.2783439065	3.9672472356	-1.4597484882
H	1.6772683297	2.9087908637	-1.5277252355
C	2.030767693	4.7570528576	-0.463712823
H	2.4029275972	5.3022435996	-1.3373917278
H	2.899397641	4.4010743766	0.1023159685
H	1.4947351486	5.4711471826	0.1721132149

C	3.4021960877	-1.7445506543	-0.6399320557
H	2.922444101	0.0301353169	-1.7404286871
H	1.8736478241	-1.3173626077	-2.1115439924
H	2.9149754058	-2.6570550839	-0.2771663412
C	4.2449895056	-1.1250554641	0.4989041725
H	4.0750165429	-2.0669710994	-1.4438983439
C	3.7127991878	-1.3913216919	1.9134007043
H	4.3365330565	-0.0426259175	0.3359340407
H	5.265940525	-1.5219695649	0.4424427556
H	3.6538646021	-2.4686012685	2.1074697659
H	2.7118123867	-0.9791003456	2.0660310471
H	4.3707630816	-0.953375788	2.671550767
H	4.3707630816	-0.953375788	2.671550767

TS endo 0694

E(RB3LYP) = -706.407232033 A.U.

First frequency = -512.9697 cm⁻¹

H	-2.0915797898	-0.2478761734	-2.1921161217
C	-1.5021637587	-0.7999812344	-1.4654777695
H	-0.7559305613	-1.4441914418	-1.9145746357
C	-2.0421570547	-1.1090602028	-0.2181060236
C	-1.1952749295	-1.7362388398	0.7223840731
C	0.0936466021	-2.1406017119	0.4258448593
H	0.7243423708	-2.5174287484	1.2250424481
H	0.3464986009	-2.5113183087	-0.5601209113
C	1.1992904431	-0.2741402063	-0.3658200459
H	1.4196549816	-0.0722361311	0.6747959599
C	2.2813586419	-0.9379151835	-1.2005702675
C	0.2473161291	0.5310836529	-0.9919210157
H	0.359637256	0.677390852	-2.0664558903
C	-0.4040338097	1.6772702442	-0.2537206748
C	-3.4922754922	-0.7106732261	0.1354919777
H	-1.4948230207	-1.7517633537	1.7653127874
C	-4.429776729	-1.6299700498	-0.6865742414
C	-3.8092792586	0.7579053388	-0.2171869323
C	-3.8147643984	-0.9103236868	1.628680791
H	-3.1780842873	-0.2878488585	2.266225476

H	-3.6942240361	-1.9535571942	1.9366534224
H	-4.8550638664	-0.6291079505	1.8224026238
H	-3.6032875187	0.9876067184	-1.2663233178
H	-3.2281054354	1.4457794273	0.402299108
H	-4.8714180831	0.9623120025	-0.0419729866
H	-5.4809933027	-1.4177277707	-0.4578329386
H	-4.2361489259	-2.6837807967	-0.461366542
H	-4.2781466755	-1.4846908227	-1.7606067925
H	-0.6261440543	1.3571079464	0.7732969501
H	-1.3627650555	1.9200993401	-0.718139674
C	0.440537119	2.9699003204	-0.222762571
H	0.6085775877	3.3116666829	-1.2541793254
C	1.7916611032	2.8651868602	0.4918090826
H	-0.1578790754	3.7550624862	0.2607076562
H	2.4287243833	2.1494323234	-0.0397259594
H	1.6395015854	2.4495825735	1.4977316835
C	2.5130982815	4.2121264876	0.594185426
H	2.6952821968	4.636947803	-0.3997868812
H	3.4811489381	4.1120626131	1.0960126787
H	1.91764707	4.9393739213	1.1580219329
C	3.2943734322	-1.8435028857	-0.4755674259
H	2.8462505785	-0.1574550034	-1.7337675217
H	1.7905703556	-1.519867029	-1.995406442
H	2.7722585072	-2.514214402	0.216431872
C	4.4288412548	-1.1241512916	0.2760583853
H	3.7590039417	-2.49191598	-1.2291253949
C	4.0131006112	-0.3483520038	1.5316829641
H	4.9421439366	-0.4445046943	-0.4183245332
H	5.17286118	-1.8786355988	0.563081577
H	3.4319484671	-0.9824051276	2.2115828981
H	3.4041670275	0.5260461749	1.2903769664
H	4.8923109881	0.0073577017	2.0792958177
H	4.8923109881	0.0073577017	2.0792958177

TS endo 0700

E(RB3LYP) = -706.406207286 A.U.

First frequency = -531.6644 cm^{-1}

H	-1.1749207584	-0.3688508539	-2.0071150754
C	-0.9682116659	-0.9187395759	-1.096421082
H	-0.1621051666	-1.6331371403	-1.1933813993
C	-1.9561605761	-1.1140380225	-0.1353734095
C	-1.5716468335	-1.7249259265	1.0782011245
C	-0.274598123	-2.1507900502	1.3234511389
H	-0.0117333879	-2.5084445007	2.3155740272
H	0.3147231023	-2.5894476176	0.5264281622
C	1.0739696234	-0.4042762251	1.0503705298
H	0.8013545434	-0.0619343976	2.0470617854
C	2.4122203907	-1.1298716057	1.0140269772
C	0.5557799415	0.3528541118	-0.0062228156
H	1.1053473425	0.3807748158	-0.938892958
C	-0.3116679837	1.5488054209	0.3258066883
C	-3.3955192016	-0.5765375104	-0.2896115444
H	-2.2606001236	-1.6864416069	1.9185232591
C	-3.8053128387	0.3635918864	0.8670370753
C	-4.3419269319	-1.8019648765	-0.2910109387
C	-3.5969250558	0.1887015207	-1.6099003978
H	-2.9545542675	1.073826825	-1.66546148
H	-4.6351007913	0.527971943	-1.6874947584
H	-3.3876174379	-0.4414212947	-2.4799449828
H	-4.2693204873	-2.3614777432	0.6465906782
H	-4.0903340289	-2.4860653726	-1.1078948566
H	-5.3837548413	-1.484629293	-0.4168705234
H	-3.2028898849	1.2760051056	0.8672727505
H	-3.6976043561	-0.1116976287	1.8456480109
H	-4.8559017182	0.6559950437	0.7585221941
H	-1.0638583837	1.2032123028	1.0442252867
H	-0.8638348321	1.8849874984	-0.5606175228
C	0.4236159939	2.7561424426	0.9540203157
H	-0.3173665544	3.3581095395	1.4970746952
C	1.1541009121	3.6886299066	-0.024869084
H	1.1328856533	2.3902461265	1.7083545282
H	1.5327079241	4.5485463202	0.5432085353
H	0.4256828523	4.096790674	-0.7392853652
C	2.3173359507	3.0564894935	-0.7970990511
H	3.010423255	2.5433457605	-0.1208197517

H	2.8841577687	3.8158461272	-1.3462077142
H	1.9646951956	2.322460422	-1.5268413573
C	2.8933107794	-1.6439387903	-0.3600663345
H	2.3755781423	-1.9721165977	1.7152026362
H	3.1714251631	-0.4521750809	1.4307231874
H	3.5054426089	-2.5420122909	-0.206582629
C	3.7205796419	-0.6443969488	-1.1900161027
H	2.0289368656	-1.9732731658	-0.9494020156
C	5.1083504734	-0.357576649	-0.6058920562
H	3.1759050041	0.2990524606	-1.2949928685
H	3.8385361194	-1.0456625653	-2.2046840425
H	5.0458661185	0.0914498541	0.3909937994
H	5.6678691343	0.3364510646	-1.2414213686
H	5.695928333	-1.2786973798	-0.516314613
H	5.695928333	-1.2786973798	-0.516314613

TS endo 0705

E(RB3LYP) = -706.406784943 A.U.

First frequency = -521.5191 cm⁻¹

H	-2.1259969322	-0.1521225909	-2.1996177733
C	-1.5207246024	-0.682673018	-1.4699623366
H	-0.7269444069	-1.2712724132	-1.9138063191
C	-2.0701262703	-1.047788846	-0.2413943565
C	-1.2104337916	-1.6400467728	0.7094403765
C	0.1060690508	-1.9679307566	0.4328010835
H	0.7424489662	-2.319015269	1.2396556477
H	0.3882946001	-2.3272744644	-0.5492954486
C	1.1252813664	-0.0637275014	-0.3264355535
H	1.361932462	0.1179720792	0.7159290663
C	2.2167897412	-0.6774305366	-1.1845217834
C	0.1410489621	0.7354278484	-0.9089043264
H	0.2410413647	0.947881749	-1.9728516651
C	-0.593146657	1.7776520453	-0.0993581534
C	-3.550168537	-0.7443290482	0.0822957714
H	-1.5302348492	-1.6861566693	1.7454143465
C	-4.4079448536	-1.7067661676	-0.7767045935
C	-3.9504161482	0.7071407954	-0.2564470058

C	-3.8953109196	-0.9883070882	1.5637784746
H	-3.3137996085	-0.3386487406	2.2264318784
H	-3.7179203967	-2.0271759326	1.8586891376
H	-4.9553159882	-0.7747214059	1.7358354248
H	-3.4342539722	1.4194400373	0.3922462544
H	-5.0283075421	0.8398001136	-0.1111251484
H	-3.7279644355	0.968943567	-1.2946125816
H	-4.1533233092	-2.7499554541	-0.5630622381
H	-4.2404966337	-1.5340068911	-1.8442865687
H	-5.4755385539	-1.5649191739	-0.5705479305
H	-0.8373501529	1.3461292928	0.8809809086
H	-1.5469336773	2.0018206161	-0.5834328863
C	0.1367079612	3.1258891009	0.1093865955
H	0.3147684854	3.5931042958	-0.8691458574
C	1.4611441275	3.0883556242	0.9012601423
H	-0.5717498195	3.7849245376	0.6277614059
H	1.4346627535	2.2595182758	1.6203689377
H	1.5418223553	4.0011896153	1.504622843
C	2.7132821004	2.9791172883	0.0239406822
H	2.8076288775	3.8588715971	-0.6230523247
H	2.6741436058	2.0982776444	-0.6197041323
H	3.6231562514	2.9108684811	0.6298694251
C	3.3129291419	-1.4271685132	-0.4133254026
H	2.6966113014	0.1127669745	-1.7815521976
H	1.7612304517	-1.3529088608	-1.9243004935
H	2.8637235483	-2.2191577235	0.1985455421
C	4.1732863033	-0.523163153	0.4799477787
H	3.9683114295	-1.9347037684	-1.1334865304
C	5.2709049806	-1.2941892962	1.2182803205
H	3.538841282	-0.0056126682	1.2100959295
H	4.6239276283	0.2658234702	-0.1368615009
H	4.8412541973	-2.066788417	1.8663645824
H	5.876324499	-0.6317884844	1.8454588799
H	5.9445359203	-1.7943920116	0.5129718573
H	5.9445359203	-1.7943920116	0.5129718573

TS endo 0712

E(RB3LYP) = -706.407071657 A.U.

First frequency = $-549.7191 \text{ cm}^{-1}$

H	-1.8356526113	-1.2458738526	-1.9737735389
C	-1.2995653258	-1.3823597935	-1.0409405375
H	-0.719401505	-2.2991037743	-1.0159589557
C	-1.8207329096	-0.8675863878	0.1505445938
C	-1.0316186608	-1.0025125815	1.3120119973
C	0.1754249212	-1.6792344582	1.3312785186
H	0.7903969943	-1.6406734024	2.2255959982
H	0.3198638511	-2.5651016139	0.7263182552
C	1.4488539235	-0.7911431664	-0.3998316863
H	1.821388332	-0.0978528802	0.3414287908
C	2.3176711112	-2.0000210939	-0.6976027702
C	0.5531711922	-0.32498242	-1.3691632831
H	0.6083738828	-0.8276347505	-2.3346312211
C	0.1736818687	1.1466079503	-1.4800021605
C	-3.1446210488	-0.0772105866	0.218899477
H	-1.2935308664	-0.4079153605	2.1846125267
C	-2.9580256879	1.3398485201	0.8055208963
C	-4.1045644192	-0.8722567875	1.1381524708
C	-3.8146272167	0.0706930264	-1.1591747854
H	-4.7596206544	0.6139138862	-1.0552046914
H	-4.0384792607	-0.9020848936	-1.6080625187
H	-3.1868638616	0.6331967656	-1.8584917969
H	-5.0750455415	-0.3673417052	1.2109490171
H	-3.6968890372	-0.9696459583	2.1488563729
H	-4.2708498489	-1.8812100013	0.7471224372
H	-3.9302902978	1.8325797755	0.9188914558
H	-2.344476892	1.9579290723	0.146894125
H	-2.4831643638	1.3225866399	1.7901818687
H	-0.8837814924	1.241788452	-1.7548900577
H	0.7354574578	1.5730067034	-2.3256564476
C	0.4437738628	2.0081331725	-0.2413059496
H	-0.0686670845	1.5750500484	0.625090181
C	0.0121486697	3.4666635128	-0.4280467584
H	1.5155853873	1.9901210614	-0.0047828789
H	-1.0447507388	3.5048162777	-0.7244534932
H	0.5730727126	3.9043062151	-1.2652518513

C	0.218432526	4.310832773	0.8323252946
H	1.2703894032	4.3093737083	1.1400762357
H	-0.3698094563	3.9142063972	1.6677499967
H	-0.0825796855	5.3517882518	0.6758019654
C	3.3732633231	-2.3356389772	0.3736198441
H	2.83230407	-1.8493947682	-1.6586595746
H	1.6710513049	-2.8755356103	-0.8632298043
H	2.9508452898	-2.1601369711	1.370838267
C	4.6981746322	-1.5652341521	0.2364571549
H	3.601547972	-3.4073516975	0.324957591
C	4.5869562472	-0.0414840573	0.3618199293
H	5.1510021001	-1.8130723668	-0.7335531159
H	5.3949691498	-1.9363880502	0.9992306537
H	3.9827849402	0.3867029248	-0.4437789943
H	5.5754527692	0.4279567752	0.3206761083
H	4.12173447	0.2444589232	1.3125620384
H	4.12173447	0.2444589232	1.3125620384

TS endo 0713

E(RB3LYP) = -706.405979471 A.U.

First frequency = -549.8632 cm^{-1}

H	-1.4087760269	-1.6181338632	-1.800488448
C	-1.1825202839	-1.5800775871	-0.7408437869
H	-0.5152429613	-2.3694172945	-0.4162738821
C	-2.092129852	-1.0263531843	0.1605005371
C	-1.6816578842	-0.9085026823	1.5047876189
C	-0.453839233	-1.3736186758	1.9504991696
H	-0.1319009114	-1.148460263	2.9639358767
H	-0.0518118391	-2.2989310936	1.5547805463
C	1.1257896527	-0.453203929	0.6559603095
H	1.1550461165	0.3913752437	1.3336650835
C	2.2249973944	-1.4740802241	0.8746062548
C	0.587866622	-0.247316018	-0.6202841107
H	1.001618766	-0.8657675335	-1.4141366056
C	0.0915705591	1.1080976157	-1.1146439835
C	-3.4508629562	-0.4362263042	-0.2728095399
H	-2.2572505185	-0.2666723142	2.1680425717

C	-3.5814396015	1.0605047604	0.0847880881
C	-4.5539982924	-1.2256601143	0.4737959209
C	-3.6995338761	-0.5812974687	-1.7850464422
H	-4.6855889503	-0.1785408691	-2.0389807913
H	-3.6757881255	-1.6289323099	-2.1011150968
H	-2.9580818195	-0.0302940732	-2.373686487
H	-4.4552457653	-1.1201718514	1.558294407
H	-4.4971233332	-2.2928285492	0.2361895485
H	-5.5478964181	-0.8621818383	0.18746729
H	-4.5907936847	1.4185741181	-0.1480062615
H	-2.8716974482	1.6607805144	-0.4886035503
H	-3.4002987096	1.2506842549	1.1459405977
H	-0.8207777766	0.95833961	-1.7010808073
H	0.8354700762	1.4800595171	-1.8365015012
C	-0.1604282871	2.2210136837	-0.0679689738
H	-1.069788855	2.7613833675	-0.3518305328
C	0.9607605179	3.2698253171	0.0489244116
H	-0.3813303827	1.7829334453	0.9119642545
H	0.6165144316	4.076880238	0.7089668532
H	1.1020443864	3.7296870597	-0.9392769559
C	2.3130049312	2.7582286432	0.5543898862
H	3.0557137401	3.5631523047	0.5624009024
H	2.6997747108	1.952534514	-0.0755962497
H	2.2366204512	2.3696228801	1.575614573
C	3.6420896189	-0.9309601763	0.5887875758
H	2.0426346619	-2.3546515999	0.2412091843
H	2.2051784719	-1.8316496353	1.9112973738
H	3.797475831	-0.0168873065	1.1783408333
C	3.9429710439	-0.6380215264	-0.8849422833
H	4.3764085911	-1.6598705358	0.9591172301
C	5.3584140064	-0.0946269546	-1.0998181596
H	3.2140961733	0.0809995408	-1.2754750489
H	3.8041352156	-1.557731063	-1.4701664252
H	5.5592813062	0.0984960288	-2.1586654149
H	6.1143567258	-0.8018677865	-0.739632187
H	5.5021323895	0.8462638217	-0.5560852249
H	5.5021323895	0.8462638217	-0.5560852249

5.2 Exo

5.2.1 Starting TS

TS exo input

E(RB3LYP) = -706.412354746 A.U.

First frequency = -497.0242 cm^{-1}

H	1.4423088835	-1.0414177784	2.1477145465
C	0.8905775916	-1.323783604	1.2546921156
H	-0.0132381351	-1.8894627536	1.4530870892
C	1.5724868961	-1.4420959965	0.0534037966
C	0.9104240398	-1.6634097145	-1.1752605257
C	-0.458535625	-1.8861427987	-1.1481513694
H	-1.0170897671	-1.9740309133	-2.0737447389
H	-0.9201823907	-2.3798278971	-0.3033091844
C	-1.3687079232	-0.0017213532	-0.0921093708
H	-1.3515128876	0.4451094587	-1.0828931352
C	-2.6959941461	-0.5678377778	0.3716178234
C	-0.4164487422	0.4255738135	0.8297396483
H	-0.7019883089	0.40935199	1.8809325168
C	0.6066170195	1.4654105679	0.4335780724
H	2.6081808855	-1.1211517187	0.0399921479
H	1.0614597951	1.1639385402	-0.5189103683
H	1.4228087886	1.4929024441	1.1659235103
C	0.0132060309	2.876236798	0.2807957842
H	-0.7991857117	2.847996193	-0.4577130274
C	1.0531877824	3.9201924563	-0.140932418
H	-0.4509109709	3.1833877072	1.228648061
H	1.5157341222	3.6046238883	-1.086437936
H	1.8642883355	3.9434439141	0.5996936666
C	0.4620873146	5.3237011688	-0.3007144162
H	-0.3294922581	5.3332263292	-1.0587735294
H	1.2230684313	6.0503776741	-0.6037152291
H	0.0210787701	5.6743288939	0.6394499948
C	-3.6624249457	-0.9314540185	-0.7621286482
H	-3.1764528706	0.1685232662	1.0304176359
H	-2.5251466176	-1.4529693129	1.0046823928
H	-3.845085704	-0.0358688888	-1.3732998707

C	-5.0067761516	-1.5031062581	-0.2864940412
H	-3.1834521115	-1.6599358075	-1.4253983385
C	-5.8695288881	-0.5137621331	0.505769743
H	-4.8210829348	-2.3979105307	0.3236851362
H	-5.5717053915	-1.8457542593	-1.1626680234
H	-5.3906411045	-0.2138203919	1.4432237554
H	-6.8405141025	-0.9513839092	0.7595434397
H	-6.0554662914	0.3964179291	-0.0764216142
C	1.6203202366	-1.4717521988	-2.5334718442
C	0.9393315221	-0.3341514864	-3.3290676346
H	1.4242671554	-0.2071618217	-4.3037345153
H	-0.1195493237	-0.5381805633	-3.5113286765
H	1.0089944256	0.6165461014	-2.7905061814
C	3.1105130369	-1.1160294544	-2.3797339766
H	3.2493985388	-0.1618242128	-1.8610682451
H	3.65672186	-1.8887335446	-1.8290478488
H	3.5725984078	-1.0247509771	-3.3681657082
C	1.5225357909	-2.7857600122	-3.3427300901
H	2.0154496744	-2.6794900196	-4.3161495036
H	2.0036246647	-3.6090746378	-2.8044645177
H	0.4810427761	-3.0686856971	-3.5214181743
H	0.4810427761	-3.0686856971	-3.5214181743

5.2.2 Lowest TS

TS exo 0004

E(RB3LYP) = -706.417083971 A.U.

First frequency = -498.6192 cm⁻¹

H	1.3726758095	-0.8461137636	-3.1100649834
C	1.3651875071	-0.0328543413	-2.389231868
H	0.8400268229	0.8539823988	-2.7255032834
C	2.3785617742	0.04616202	-1.4481973464
C	2.3648200796	0.9782949632	-0.3843655047
C	1.3274941558	1.8991023153	-0.3488954122
H	1.205422912	2.5815231785	0.4834903925
H	0.8982836487	2.2581629362	-1.2753128324
C	-0.581045111	0.6596136605	-0.2658494522

H	-0.3895984442	0.5080592568	0.792827817
C	-1.560672265	1.7622133209	-0.6151026995
C	-0.4220638064	-0.4440095312	-1.1054929199
H	-1.025658965	-0.4591875756	-2.0114263146
C	-0.0384296772	-1.7935159477	-0.5320173126
H	3.077358825	-0.7850854969	-1.3944053933
H	0.8850515915	-1.6776669299	0.0459504619
H	0.1913204537	-2.4922601277	-1.3461067889
C	-1.1155314217	-2.4109506616	0.3822701131
H	-0.7347072666	-3.3557860297	0.7950135275
C	-2.4584321608	-2.6694859207	-0.3091946514
H	-1.2768718328	-1.7461868189	1.2417331407
H	-2.3047020031	-3.3568097119	-1.1526339983
H	-2.8283790267	-1.7325192984	-0.7422451696
C	-3.5162442801	-3.2379012805	0.6403567299
H	-3.1847937711	-4.183621678	1.0845014479
H	-4.463519833	-3.4253469335	0.1239159635
H	-3.7181690167	-2.5400915076	1.4611715615
C	-3.0388538637	1.3411328767	-0.482000458
H	-1.3872206041	2.0857213909	-1.6509956829
H	-1.3783403755	2.640999116	0.0161529124
H	-3.6784724886	2.1797014129	-0.7912789044
C	-3.4425309006	0.8938433287	0.9270738085
H	-3.2393574349	0.525082312	-1.1889865658
C	-4.9061454453	0.4527032583	1.0113570026
H	-3.2575333481	1.714008565	1.6345570767
H	-2.7977795548	0.0653191733	1.2429518766
H	-5.5833477963	1.2617296391	0.7141628204
H	-5.1767822988	0.1467027014	2.0272859711
H	-5.0953158799	-0.398241461	0.3470052449
C	3.3544184831	0.7949277639	0.7842619303
C	3.1340506265	-0.5718973215	1.4738704415
H	3.2728488139	-1.4047031872	0.7787579235
H	3.8426070857	-0.7052971628	2.2996094726
H	2.1208455579	-0.6410754101	1.8835352128
C	4.7960860138	0.8592001993	0.2296246555
H	4.9850993439	1.8254442082	-0.2491135689
H	5.5234740843	0.7300000635	1.0393186407

H	4.9820744702	0.077478528	-0.5124504159
C	3.2046282766	1.893882972	1.8523847551
H	3.3459361703	2.8919959925	1.4256545583
H	2.2206106508	1.8627676159	2.331693569
H	3.9555702374	1.7547014488	2.6370330453
H	3.9555702374	1.7547014488	2.6370330453

5.2.3 Additional TS

TS_{exo} 0001

E(RB3LYP) = -706.415654804 A.U.

First frequency = -501.1935 cm⁻¹

H	1.0208337039	-0.4647028386	-3.2539801737
C	1.1042725758	0.2306163663	-2.4229201352
H	0.6155184778	1.1835838235	-2.5905310191
C	2.1741259451	0.1167066286	-1.5504697919
C	2.2778900609	0.8796983926	-0.364197415
C	1.2959233683	1.8291319702	-0.1221401051
H	1.261177185	2.3820648686	0.8087855039
H	0.8263093417	2.3411230077	-0.9523395737
C	-0.6666812239	0.6723388084	-0.0889054593
H	-0.4198310617	0.342641953	0.9181415272
C	-1.6171030732	1.8453452636	-0.1768506678
C	-0.6210058322	-0.2875006584	-1.1013738612
H	-1.2859228756	-0.1350127652	-1.9514815176
C	-0.2919486809	-1.7266232161	-0.7725839787
H	2.8225730992	-0.7486344982	-1.6639972549
H	0.5947025448	-1.748935481	-0.1275499831
H	-0.0229594575	-2.2756370999	-1.6833925223
C	-1.4465371018	-2.4565696713	-0.064568867
H	-1.7067890624	-1.9121092076	0.8531982341
C	-1.1168360851	-3.9136146131	0.2779958862
H	-2.3438246285	-2.4231093279	-0.6988617936
H	-0.2165666532	-3.9399399056	0.9073243661
H	-0.8578207614	-4.4527991941	-0.6435004292
C	-2.2642707521	-4.6349865181	0.990720145
H	-3.1667839012	-4.6491495177	0.3689258021

H	-2.5208058786	-4.1330769877	1.9307399398
H	-2.0050079682	-5.6724392222	1.2262533866
C	-3.0535162394	1.4697691647	0.2292123677
H	-1.6272587464	2.2314103015	-1.2064920768
H	-1.2735969685	2.6723024224	0.457730917
H	-3.408223955	0.6591633486	-0.4212617534
C	-4.0300455185	2.6492685517	0.1660453353
H	-3.0435493617	1.0567450771	1.247795604
C	-5.4567546411	2.2648286617	0.5683932805
H	-4.0324373172	3.0614858571	-0.8523921464
H	-3.667199358	3.4552508307	0.8184631643
H	-5.4859867477	1.8793740777	1.5939797426
H	-5.8533606221	1.4821594233	-0.0883784951
H	-6.1360363523	3.1218719978	0.5144413346
C	3.3216810738	0.4742806279	0.6963012072
C	4.7289130229	0.5322477129	0.0589190305
H	5.4925874977	0.2477321982	0.7918895016
H	4.8183767435	-0.1460565955	-0.794400018
H	4.9536631411	1.5438887481	-0.294087167
C	3.3113432687	1.4165095813	1.9141374962
H	4.0995886697	1.125724365	2.6163844744
H	3.4897662718	2.4557352874	1.620005912
H	2.3597846723	1.3725068379	2.454067202
C	3.0496309313	-0.961766302	1.2025080869
H	2.0626107219	-1.0265125507	1.6725008524
H	3.0824222467	-1.6922383466	0.3892841969
H	3.7983900377	-1.2564940494	1.9469937305
H	3.7983900377	-1.2564940494	1.9469937305

TS exo 0005

E(RB3LYP) = -706.415918996 A.U.

First frequency = -500.0603 cm⁻¹

H	1.2826460004	-0.5543844324	-3.2519698516
C	1.3079407519	0.1950821413	-2.465335925
H	0.8833582443	1.1511887961	-2.7498695095
C	2.2746185506	0.1052333317	-1.477013563
C	2.2872150261	0.9478158967	-0.3412292926

C	1.3309035661	1.950166227	-0.2729698758
H	1.2223454122	2.5697271593	0.6090014945
H	0.9749394671	2.4172921517	-1.1822271611
C	-0.6766778866	0.8666306847	-0.3772254225
H	-0.5415535698	0.6036438505	0.6684356713
C	-1.5545015854	2.0680523338	-0.6573519994
C	-0.5653568476	-0.1646422261	-1.3115606333
H	-1.1305387106	-0.0501100022	-2.2366168198
C	-0.3385615408	-1.5883332602	-0.8536128836
H	2.8919759628	-0.7896134494	-1.4607843931
H	0.4759684174	-1.5998122415	-0.1194833158
H	-0.0049196153	-2.2111840221	-1.6927849406
C	-1.5919863131	-2.2195070388	-0.2229986081
H	-1.909587964	-1.6087748647	0.6328494026
C	-1.3744483818	-3.6659540333	0.2342634749
H	-2.4219788398	-2.1831113321	-0.9429097422
H	-0.5390611205	-3.6957483364	0.9473014062
H	-1.0611290542	-4.2745541013	-0.6249971165
C	-2.6207253747	-4.2831680609	0.8752519141
H	-3.4612462371	-4.2927084279	0.1718422733
H	-2.935190617	-3.7099830972	1.7550035392
H	-2.4417674908	-5.3148534005	1.1954619078
C	-3.0591774774	1.7795647758	-0.4772294127
H	-1.383017706	2.403016194	-1.6897622807
H	-1.2735174343	2.9083554832	-0.0096964481
H	-3.6331456628	2.6594384117	-0.8004291496
C	-3.4585565595	1.4238302979	0.9594340389
H	-3.3456351119	0.9568878985	-1.1462122576
C	-4.9586689832	1.1560290682	1.1081511924
H	-3.1587089427	2.2412060083	1.6300482275
H	-2.8978216869	0.53935706	1.2857481216
H	-5.5482637594	2.0317234455	0.8131465423
H	-5.2236290916	0.9077236853	2.1411308408
H	-5.2715307274	0.3191994019	0.4731929988
C	3.1915198214	0.5792173053	0.8524888934
C	2.796934554	-0.8033642217	1.422868926
H	3.4457145361	-1.0727498891	2.2644457085
H	1.7629550938	-0.7929771236	1.7836115131

H	2.8817673682	-1.5924355614	0.6704083813
C	4.6597737474	0.5322225872	0.3710203673
H	4.9701644959	1.5051307998	-0.0235084517
H	5.32604519	0.2709810183	1.201200283
H	4.8065543087	-0.2099492132	-0.4188497674
C	3.0973190031	1.6079693743	1.9942888342
H	2.0928093139	1.6422496217	2.428686956
H	3.7916125933	1.3379353403	2.7968153217
H	3.3557163741	2.6146863725	1.6506791855
H	3.3557163741	2.6146863725	1.6506791855

TS exo 0009

E(RB3LYP) = -706.415675432 A.U.

First frequency = -510.2487 cm⁻¹

H	0.8145489435	-0.4560597068	-3.2295216605
C	1.0097292878	0.2480745446	-2.4248223937
H	0.6387164136	1.2489757719	-2.6139516571
C	2.095558122	0.0328080854	-1.5891892504
C	2.3330290821	0.8103089584	-0.4336061251
C	1.4751516918	1.8742526528	-0.190466554
H	1.5374355325	2.4533982598	0.723043892
H	1.0453889008	2.4168406815	-1.0227811968
C	-0.6126676088	0.9784615438	-0.0666391263
H	-0.3797103125	0.6614095133	0.9482258764
C	-1.4083836362	2.2623929361	-0.1717713899
C	-0.6976901109	-0.0240971767	-1.0382224537
H	-1.3703258457	0.1578464968	-1.8749134154
C	-0.4997031294	-1.4729768376	-0.647283421
H	2.6324812128	-0.9064968035	-1.697521905
H	0.4029434731	-1.5481304231	-0.0294212319
H	-0.3129297421	-2.0861850921	-1.5373516883
C	-1.686739053	-2.0656586741	0.1314386234
H	-1.8863685963	-1.4438500415	1.0147049882
C	-1.4532776301	-3.5161377695	0.5683271823
H	-2.5940135295	-2.0139732387	-0.4869012913
H	-0.54518146	-3.563718101	1.1849606299
H	-1.2504485437	-4.1332634281	-0.3176288573

C	-2.6350323428	-4.103493307	1.345069086
H	-2.8380199955	-3.5216321348	2.2514948005
H	-2.4449771575	-5.1383124038	1.6482860565
H	-3.5477855384	-4.095408945	0.7383055476
C	-2.8195527325	2.172971885	0.4482634926
H	-1.4978097066	2.5501207608	-1.2291862433
H	-0.873372388	3.0810404598	0.3245712975
H	-2.7301052829	1.8311692976	1.4893574518
C	-3.7977158046	1.2620391574	-0.3004325928
H	-3.2434472692	3.1857708823	0.4970179824
C	-5.1867414432	1.2302734765	0.3435067215
H	-3.3911778078	0.2463872106	-0.3429207124
H	-3.8800398711	1.6026684996	-1.3421144738
H	-5.1327843944	0.8607369501	1.3741010907
H	-5.8708512613	0.5772221643	-0.2082660181
H	-5.6332705145	2.2308549794	0.3758669848
C	3.3692128852	0.3227703126	0.5996226658
C	3.5128917024	1.2965272836	1.7837399547
H	4.2925294591	0.941119662	2.4655724216
H	3.7923547393	2.3000465102	1.4473720671
H	2.5851696815	1.3749848275	2.3600316106
C	2.9665776898	-1.0591395727	1.1654678169
H	2.0029585028	-1.000727242	1.682469644
H	2.8794862026	-1.8116278521	0.3766718487
H	3.7142196527	-1.4137425817	1.8845205574
C	4.7458309675	0.2070680358	-0.0944640898
H	5.5052700842	-0.1364769693	0.6173262887
H	4.7243159404	-0.5028968131	-0.9262101932
H	5.0629230456	1.176715041	-0.491652692
H	5.0629230456	1.176715041	-0.491652692

TS exo 0010

E(RB3LYP) = -706.415218868 A.U.

First frequency = -512.6820 cm^{-1}

H	1.1334161837	-0.2166470968	-3.3429674902
C	1.1746345808	0.3888781598	-2.4412710442
H	0.623422356	1.3201644809	-2.5092129213

C	2.2631080537	0.2613253117	-1.59154701
C	2.3235311338	0.9002474278	-0.3330258825
C	1.2759185497	1.7450898885	0.0073872882
H	1.2077227692	2.1918521545	0.9920709156
H	0.7727984408	2.3130400971	-0.7648469868
C	-0.5939141207	0.4607381591	-0.092619969
H	-0.327323449	0.062003912	0.8823754827
C	-1.6183779819	1.5747456505	-0.0929247187
C	-0.4812813878	-0.3975599319	-1.1911274635
H	-1.1625927161	-0.2117344662	-2.0223686922
C	-0.0469327146	-1.839904167	-1.0299419349
H	2.9693384049	-0.5389854762	-1.7986602061
H	0.7576835048	-1.8898538795	-0.2866440247
H	0.3835217743	-2.203532836	-1.9698338696
C	-1.1828056185	-2.800409837	-0.6174578221
H	-2.0168944193	-2.6986245912	-1.3267393943
C	-1.708972675	-2.6156825243	0.8099327775
H	-0.8182159294	-3.8316230183	-0.7267233971
H	-2.1132071353	-1.6048037538	0.9242559397
H	-0.8689102735	-2.6913193291	1.5146826813
C	-2.7864357887	-3.6394372009	1.1792122606
H	-2.4037380937	-4.6638957448	1.1042749673
H	-3.6488004928	-3.56078781	0.5070152958
H	-3.1480953625	-3.4921773985	2.2022486014
C	-3.0370806551	1.088165929	0.2529710847
H	-1.6389036857	2.0475262487	-1.0858050402
H	-1.3337145337	2.363143906	0.6153983052
H	-3.3284899863	0.3000265631	-0.4542430879
C	-4.0831015293	2.2082162112	0.2372432769
H	-3.0250566826	0.6163458912	1.2454835217
C	-5.4901942507	1.7138766923	0.5849042502
H	-4.0920300116	2.6794555627	-0.7551828821
H	-3.782874268	2.9941733579	0.9436298408
H	-5.824863373	0.9487810985	-0.1249162887
H	-6.220543693	2.5293544581	0.5659013642
H	-5.5141971128	1.2670108816	1.5853917608
C	3.3975202783	0.4574188253	0.6810802187
C	4.7947063566	0.6580830297	0.050887441

H	4.9580029876	1.7101324858	-0.2042432522
H	5.5781104968	0.350398224	0.7529941914
H	4.9188166222	0.0703387412	-0.8630721133
C	3.3410852796	1.2761406154	1.9840294828
H	3.4517921111	2.3478565623	1.790272298
H	2.3995245607	1.121235882	2.5209827369
H	4.1524833118	0.969125763	2.6521951015
C	3.2109707081	-1.0339692245	1.0458572745
H	3.2752266022	-1.6780495356	0.164351563
H	3.982167779	-1.3575148936	1.7546388334
H	2.2337167557	-1.199162539	1.5117551486
H	2.2337167557	-1.199162539	1.5117551486

TS_{exo} 0012

E(RB3LYP) = -706.415970250 A.U.

First frequency = -517.6384 cm⁻¹

H	0.9861245657	-0.0109912785	-3.3293601142
C	1.1127280026	0.5661664404	-2.4169925126
H	0.6564945584	1.5491408736	-2.450587442
C	2.2113681766	0.3153955635	-1.6071578089
C	2.3700892407	0.9144635653	-0.3386695679
C	1.4144366887	1.8427452504	0.0537642184
H	1.4179243337	2.2688986534	1.0499201647
H	0.9454569533	2.4757235037	-0.6890155576
C	-0.5640544334	0.7449214463	-0.0054484954
H	-0.2945619183	0.2875462833	0.9431190111
C	-1.4828548737	1.9456341136	0.0986933643
C	-0.5646257017	-0.0851070038	-1.1338215622
H	-1.2493976341	0.1871849267	-1.9363301114
C	-0.2644676218	-1.5672222727	-1.022138019
H	2.8305859501	-0.5435496419	-1.8541030724
H	0.5605678381	-1.7128488646	-0.3147488443
H	0.091858825	-1.9441709791	-1.9873105111
C	-1.4704674774	-2.4276071176	-0.5855095642
H	-2.3263148743	-2.2041538304	-1.2386597102
C	-1.8934106219	-2.2679849653	0.8791558645
H	-1.2265226137	-3.4842355192	-0.7642303362

H	-2.1069146786	-1.2158758802	1.0914594167
H	-1.0495291651	-2.5440631445	1.5265636519
C	-3.1208936053	-3.1115407853	1.2348545851
H	-2.9417153371	-4.1764505371	1.046659851
H	-3.9872066764	-2.8113417203	0.6338921762
H	-3.3938119073	-3.0000994188	2.2894764414
C	-2.8816606804	1.6115891547	0.6634294248
H	-1.5952260091	2.4077486187	-0.8926525335
H	-1.0322160789	2.7095241772	0.7434616971
H	-2.7600078184	1.0635532007	1.6086723545
C	-3.7849659853	0.8081313992	-0.2783539328
H	-3.3900782233	2.5503222217	0.9237023696
C	-5.1184155939	0.4219326605	0.3675894595
H	-3.265317827	-0.0986657044	-0.6030595233
H	-3.9668811582	1.3970691183	-1.1879249134
H	-4.9561078531	-0.2150661682	1.2448296567
H	-5.7578174517	-0.1296465379	-0.3294885802
H	-5.6724624493	1.3073385051	0.7002228148
C	3.4283838019	0.3501064644	0.6306235393
C	4.8183126816	0.4358836284	-0.0403214466
H	5.5906542187	0.0397609039	0.6289457036
H	4.8588386527	-0.1381895065	-0.9703759869
H	5.0712857506	1.4742027736	-0.2778929401
C	3.4878943667	1.1392638127	1.951567661
H	4.2874294329	0.7431166471	2.5862977728
H	3.6914794674	2.2005549642	1.7766768823
H	2.5529579938	1.0590264313	2.5157742662
C	3.1152733648	-1.1260529267	0.9698370982
H	3.0936755613	-1.7520672504	0.0733509033
H	3.8738655321	-1.5359967262	1.6468160785
H	2.1411848392	-1.2120269573	1.4629484983
H	2.1411848392	-1.2120269573	1.4629484983

TS exo 0014

E(RB3LYP) = -706.415498986 A.U.

First frequency = -480.6123 cm⁻¹

H	1.0043268709	-0.2043767027	-3.3462540094
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C	1.0859883157	0.4165056679	-2.4582123558
H	0.5715689408	1.3674602276	-2.5287984642
C	2.1500024175	0.2255758477	-1.5943626588
C	2.2468037596	0.8826275839	-0.3457562906
C	1.2713216572	1.818038318	-0.0302874278
H	1.2425940945	2.280823739	0.9514175124
H	0.8102775734	2.4116427169	-0.8090289558
C	-0.7038490521	0.6711910007	-0.0833762207
H	-0.4563617787	0.3047809605	0.9103528355
C	-1.6545717389	1.8457608723	-0.1304881997
C	-0.6417227902	-0.2423558672	-1.1324431116
H	-1.2988355476	-0.0710734592	-1.9840928881
C	-0.2408445191	-1.6753396749	-0.8702013442
H	2.7982653713	-0.6216289566	-1.7898570595
H	0.67044613	-1.6786614144	-0.2573684489
H	0.0211082814	-2.1773330138	-1.8095475962
C	-1.3330751549	-2.4843195922	-0.1489914826
H	-1.5891419035	-1.9823440644	0.7937198443
C	-0.9192345591	-3.9322808914	0.1356050029
H	-2.2514742134	-2.4771063974	-0.752923269
H	0.0013163959	-3.9314272679	0.7356291115
H	-0.6634087381	-4.4288364368	-0.8104038185
C	-2.0046924583	-4.7334738223	0.8600100648
H	-2.9252076679	-4.7749961556	0.2664993133
H	-2.2552629673	-4.2746987326	1.8233785668
H	-1.6856674407	-5.7629254921	1.0534780825
C	-3.0923882983	1.4537859045	0.2545028837
H	-1.659855599	2.272239229	-1.1440517863
H	-1.3140518626	2.6467882647	0.538077629
H	-3.4442415239	0.6702095929	-0.4297630214
C	-4.0689545017	2.6347339391	0.2357370875
H	-3.0859938327	0.9997559086	1.2554942808
C	-5.4969985704	2.2343164915	0.6172423617
H	-4.0678640779	3.0880007023	-0.7651019472
H	-3.7085123521	3.4135431838	0.921645137
H	-6.1761009833	3.0929305356	0.5960007438
H	-5.5296812132	1.8073705727	1.626162723
H	-5.8913942669	1.4791467518	-0.0722404248

C	3.2493208867	0.434091644	0.7388596735
C	4.1975240762	-0.6753909942	0.248002916
H	4.9151399388	-0.9238362406	1.0367321713
H	3.6553940342	-1.5924570756	-0.0044883916
H	4.7674197758	-0.3602202809	-0.6321314599
C	4.1109469606	1.6455060483	1.1640873767
H	4.6711781374	2.0412328382	0.3105428077
H	3.4938711473	2.4564099156	1.5618624266
H	4.8292983188	1.3567367004	1.9401910276
C	2.4837493474	-0.1026859947	1.9704235299
H	1.8734896502	-0.9716016846	1.7028430054
H	3.1863408686	-0.4100632582	2.7535102121
H	1.8198777619	0.6529221938	2.4003505673
H	1.8198777619	0.6529221938	2.4003505673

TS exo 0015

E(RB3LYP) = -706.417041371 A.U.

First frequency = -473.7528 cm⁻¹

H	1.3371062742	-0.9153211974	-3.1934658003
C	1.3597534542	-0.1029547915	-2.4722546246
H	0.8341490717	0.7906038356	-2.7874133218
C	2.3718671937	-0.0607696458	-1.5305815176
C	2.3884044378	0.870474782	-0.4654877649
C	1.3914048364	1.8353879487	-0.4330744114
H	1.3035806288	2.5143011749	0.4095095827
H	0.9756697004	2.2223239613	-1.3542364572
C	-0.5662535701	0.6684191752	-0.3185174235
H	-0.3651850528	0.5528101884	0.742561697
C	-1.5159993058	1.7856522892	-0.6997647891
C	-0.4449117524	-0.4666278263	-1.1148396617
H	-1.0466319001	-0.5065117255	-2.0205511805
C	-0.0494159375	-1.7923438728	-0.4999359039
H	3.0416992527	-0.9126799402	-1.4882830672
H	0.8971197204	-1.6585262127	0.0388515151
H	0.1466798229	-2.5274512159	-1.2902115232
C	-1.0976172838	-2.3585291508	0.4794081686
H	-0.7126068993	-3.2901727728	0.9174022596

C	-2.4676217033	-2.6271195608	-0.1527852364
H	-1.2202841969	-1.6562881356	1.3151197302
H	-2.3531092227	-3.3523050096	-0.9703488849
H	-2.839502059	-1.7038808031	-0.6131527403
C	-3.4987204425	-3.1380059791	0.8568575082
H	-3.164602374	-4.0683595049	1.3304832767
H	-4.4659541228	-3.3335121764	0.3821360281
H	-3.6623045114	-2.4022542384	1.652766492
C	-3.0024076562	1.4075931727	-0.5314338102
H	-1.3466283561	2.0647339153	-1.749054389
H	-1.3015132519	2.6817344834	-0.1039293124
H	-3.6265913176	2.2497717039	-0.8615344708
C	-3.3947935834	1.019979841	0.8986019001
H	-3.2322532383	0.5714493073	-1.2053861305
C	-4.8657370985	0.6130480255	1.0191673472
H	-3.1824390495	1.8608402935	1.5733495405
H	-2.7628944206	0.1896772006	1.2353026489
H	-5.0817935608	-0.2574077138	0.3890889688
H	-5.5306769274	1.424579543	0.7018127223
H	-5.1276654296	0.3498753033	2.0492576086
C	3.3233916025	0.7039404211	0.7513976151
C	2.4827575539	0.4381812947	2.0218286456
H	1.7851885854	1.2551402871	2.2281826884
H	1.89899515	-0.4823683405	1.9182461956
H	3.1344534284	0.3303987658	2.8964700297
C	4.3144369863	-0.462509227	0.5835534745
H	4.9827299709	-0.5069639199	1.4496818194
H	3.8013880721	-1.4272230763	0.5145615934
H	4.9358987916	-0.3396422518	-0.3094628388
C	4.1420783383	2.0012210493	0.9450832581
H	3.4921876546	2.8651857712	1.1114917895
H	4.8106021745	1.9116096365	1.8091987841
H	4.7533403084	2.2095149223	0.0607980843
H	4.7533403084	2.2095149223	0.0607980843

TS exo 0020

E(RB3LYP) = -706.415695884 A.U.

First frequency = -479.4873 cm^{-1}

H	1.1474134411	-0.7267756002	-3.2060880371
C	1.1967939635	0.022679687	-2.4208902738
H	0.5975707552	0.9059084129	-2.6067612733
C	2.2935773506	0.0499789687	-1.5782089433
C	2.3629718652	0.8882927308	-0.441117699
C	1.3162806017	1.7742010323	-0.2259513832
H	1.2728735872	2.3719162911	0.6793498261
H	0.7866218824	2.2082936351	-1.0640867752
C	-0.5477124762	0.4767283552	-0.0343169508
H	-0.2443100504	0.2763322463	0.9908337738
C	-1.5968223886	1.5523502237	-0.2054527454
C	-0.4398990038	-0.5706036031	-0.9456926309
H	-1.1251079772	-0.5682653704	-1.7910903928
C	0.0892043495	-1.9156442896	-0.4979026781
H	3.0097592838	-0.7587676208	-1.6742239451
H	1.0359724896	-1.7552046684	0.0330802822
H	0.3265458691	-2.5379726336	-1.369520978
C	-0.8780983301	-2.6817874947	0.4262284845
H	-0.381569915	-3.5934313681	0.7876188262
C	-2.203882338	-3.064563063	-0.2410261741
H	-1.0858872214	-2.069211696	1.31405699
H	-1.9964809317	-3.6718823768	-1.1331655307
H	-2.7043841922	-2.1564222513	-0.5997319896
C	-3.1437239314	-3.8265867662	0.6970017234
H	-2.6799564251	-4.7531769237	1.0546603596
H	-4.0820749896	-4.0934380777	0.1996640987
H	-3.3927620742	-3.2223984933	1.5770281962
C	-2.984492539	1.1031018711	0.2862980902
H	-1.6669613934	1.8313094478	-1.2667399519
H	-1.3078427329	2.4637331516	0.3335108086
H	-3.2943498223	0.2148754358	-0.280221063
C	-4.0558005487	2.1918676295	0.1626614096
H	-2.9085575282	0.7810129008	1.3344310793
C	-5.4330608239	1.7298891335	0.6473864623
H	-4.1227234017	2.5150853542	-0.8852578718
H	-3.7409704995	3.0762036558	0.7333584617
H	-6.1821873908	2.5223183091	0.5491345533
H	-5.3992349026	1.4307923536	1.7012639376

H	-5.7832198453	0.8655885266	0.0715277114
C	3.4286901515	0.6893754671	0.6576068934
C	2.745202411	0.2709274762	1.9798907381
H	2.2093375349	-0.6763197195	1.8596513191
H	3.4915315187	0.140548121	2.7719296671
H	2.0265348801	1.0206678469	2.3233216002
C	4.4623527443	-0.3920590195	0.292917402
H	5.2194306521	-0.46023101	1.0809438506
H	4.0012946224	-1.3800919223	0.193584375
H	4.9784299687	-0.1584551419	-0.6440246064
C	4.1863866012	2.0195736624	0.8754203894
H	4.9470000522	1.9084858072	1.6569695326
H	4.6870055185	2.3358422856	-0.0456435695
H	3.5081950281	2.8226659468	1.1781475512
H	3.5081950281	2.8226659468	1.1781475512

TS exo 0029

E(RB3LYP) = -706.415658541 A.U.

First frequency = -488.3650 cm⁻¹

H	0.8484066965	-0.1769169059	-3.3271265054
C	1.0302468415	0.4530683625	-2.4604741351
H	0.63265815	1.457064096	-2.5483643924
C	2.0966974854	0.1620901151	-1.6259410924
C	2.3092185198	0.833147853	-0.4004917571
C	1.4556308417	1.8817610581	-0.08438729
H	1.5098923923	2.3694030977	0.8841974574
H	1.0472428109	2.5070069518	-0.8677703977
C	-0.639666184	0.9836643094	-0.0504121667
H	-0.4081518136	0.6200419559	0.9487529501
C	-1.4452036431	2.2642131432	-0.0996327906
C	-0.703696843	0.033990834	-1.0700596439
H	-1.3643210296	0.2435761488	-1.9090208547
C	-0.4427824669	-1.4232773939	-0.7628753487
H	2.6350668954	-0.7598666784	-1.8168234624
H	0.4815485402	-1.4955243608	-0.1745133189
H	-0.2586826803	-1.9813650356	-1.6888425922
C	-1.5835975055	-2.0996886822	0.0171776081

H	-1.779696466	-1.5312181557	0.9362899694
C	-1.2843291644	-3.5603453634	0.3720284993
H	-2.5098127557	-2.0506063178	-0.572556013
H	-0.3576067948	-3.6040857961	0.960804497
H	-1.0844239387	-4.1237296178	-0.5496583593
C	-2.4203831727	-4.2311648758	1.1493050377
H	-2.1833162888	-5.2718661993	1.3934891214
H	-3.3500064785	-4.2276502383	0.5687031621
H	-2.6182984855	-3.7039981538	2.0896543646
C	-2.8553962103	2.1314261794	0.5146019793
H	-1.5365342559	2.5977645995	-1.1432450644
H	-0.9183331113	3.0646610449	0.4338169788
H	-2.7612437472	1.7598730022	1.5450429583
C	-3.8149597264	1.2247507686	-0.2629406845
H	-3.297647234	3.1344242883	0.5929173211
C	-5.2054121259	1.1510603671	0.3744312586
H	-3.3898490877	0.2178755684	-0.3321811605
H	-3.8996925297	1.5924209811	-1.2952039993
H	-5.8757468543	0.5007962034	-0.1971775314
H	-5.6699624671	2.1422862558	0.4314571663
H	-5.1485341911	0.7553878497	1.3951212085
C	3.2902504905	0.3016724246	0.6658619598
C	2.5125560854	-0.106812378	1.9383546902
H	3.2030577509	-0.4694518746	2.7084223314
H	1.9546172969	0.7322954697	2.3638213635
H	1.7984014874	-0.9075182966	1.7198811313
C	4.08601939	-0.9239851022	0.1809627363
H	4.6578119667	-0.7018442051	-0.7259261091
H	4.7968959303	-1.2328997959	0.9542885748
H	3.4328368667	-1.7779807357	-0.0258398452
C	4.2999701199	1.4166461055	1.0238991169
H	3.7942290839	2.3043474796	1.4148576046
H	5.0076208474	1.0688590456	1.7854923241
H	4.8711425319	1.7205721787	0.1405109986
H	4.8711425319	1.7205721787	0.1405109986

TS exo 0033

E(RB3LYP) = -706.415098330 A.U.

First frequency = $-491.7416 \text{ cm}^{-1}$

H	1.1312985364	0.0507293133	-3.4119533146
C	1.1711740318	0.5814034076	-2.4644170972
H	0.5945665729	1.4987024969	-2.4432601903
C	2.2531611003	0.3822269999	-1.6229362697
C	2.3069029621	0.9159593803	-0.3158317518
C	1.2637238181	1.7389722191	0.0874402177
H	1.2023084573	2.0955228571	1.1111587591
H	0.7631761837	2.3770945248	-0.6293455978
C	-0.6131551587	0.4619922696	-0.0986760764
H	-0.3388294235	0.02220681	0.8559487244
C	-1.6442287906	1.5678401007	-0.045567357
C	-0.4891452619	-0.3384349657	-1.2341747008
H	-1.1627895497	-0.1252703632	-2.0642795514
C	0.0073619149	-1.765197287	-1.1472835728
H	2.9598512104	-0.3917900981	-1.9017290068
H	0.8319247688	-1.8102054387	-0.4239927459
H	0.4316939595	-2.0685715657	-2.1108765374
C	-1.0743967445	-2.7928576578	-0.7512343402
H	-1.9192897259	-2.7141856239	-1.4504191488
C	-1.5964518947	-2.6746129909	0.6848093278
H	-0.6584768396	-3.8004899851	-0.8927206252
H	-2.0632494942	-1.6943573049	0.8261385453
H	-0.7465029927	-2.7120620145	1.3807793516
C	-2.6024359052	-3.773679652	1.0390595799
H	-3.4734900602	-3.7371294847	0.3745085115
H	-2.964545184	-3.6716297008	2.0674178696
H	-2.1548646836	-4.7693526891	0.9396448721
C	-3.057221534	1.0525642299	0.2819099523
H	-1.6713217862	2.0865811968	-1.0149627555
H	-1.3629998633	2.3237630447	0.698640006
H	-3.3457441199	0.2997695469	-0.4639344262
C	-4.112368638	2.1630177832	0.3298906304
H	-3.0354229948	0.5294941855	1.2483001498
C	-5.5135845471	1.6396206342	0.6582246775
H	-4.1303874412	2.6853622161	-0.6364842359
H	-3.8146806863	2.9134724161	1.0749152929

H	-5.5285769728	1.1408147571	1.6340411859
H	-5.8460788627	0.9100385564	-0.0890179909
H	-6.2504566244	2.4489663295	0.685670035
C	3.3407685506	0.4339129671	0.7236035055
C	4.3702046366	-0.543277909	0.1268514175
H	4.9127353171	-0.0958423392	-0.712348611
H	5.1059953379	-0.8168622402	0.890124101
H	3.8994687261	-1.4677918125	-0.2227736444
C	4.1081058694	1.6557087998	1.2796109852
H	4.6370225155	2.1794178475	0.4764988501
H	3.4314555522	2.3719269497	1.7547548974
H	4.8460437644	1.3423017405	2.0272396555
C	2.6176389491	-0.284380438	1.8864260208
H	1.8987290342	0.3704822475	2.3872566882
H	2.0742469036	-1.1636171052	1.5250466484
H	3.3412019337	-0.6186357673	2.6387984226
H	3.3412019337	-0.6186357673	2.6387984226

TS exo 0037

E(RB3LYP) = -706.415011516 A.U.

First frequency = -501.7573 cm^{-1}

H	0.9448001776	-0.6535523371	-3.1119549103
C	1.0048250999	0.0813862384	-2.3136519466
H	0.378534708	0.9531607784	-2.4643802438
C	2.1511480749	0.1471483773	-1.53900356
C	2.2518030803	0.9655777125	-0.3900817423
C	1.173311428	1.7844956224	-0.0874570022
H	1.1444627238	2.3666814627	0.8256578934
H	0.5702341611	2.1959951164	-0.8868031283
C	-0.6025403703	0.3866414987	0.1602274332
H	-0.2312631194	0.1325517501	1.1510082829
C	-1.7045184287	1.4220755084	0.1242184622
C	-0.5172971482	-0.6007031884	-0.8233709719
H	-1.2611837179	-0.5646230565	-1.6176558828
C	0.0346575251	-1.9688061605	-0.4803814094
H	2.899721223	-0.6276149032	-1.6859064681
H	0.9880321532	-1.8366640896	0.0433335245

H	0.2603863328	-2.5271495787	-1.3974444052
C	-0.9090916427	-2.8078908828	0.4037548746
H	-0.3937507546	-3.7324864504	0.700052057
C	-2.2372645746	-3.1708934758	-0.2699522157
H	-1.1146207193	-2.2565101951	1.3314298062
H	-2.0315519696	-3.7188411341	-1.2001099143
H	-2.758088006	-2.2518544181	-0.5664800272
C	-3.1522394221	-4.0049629457	0.6306778805
H	-4.0923978681	-4.2573113188	0.1291845815
H	-3.3997365777	-3.4599918317	1.5489758612
H	-2.6684405311	-4.9433802893	0.9254146069
C	-3.030145939	0.881152933	0.6941202857
H	-1.8553194521	1.7493247986	-0.9129335298
H	-1.4172313911	2.3168418076	0.6919057875
H	-3.3573368271	0.0277608079	0.0851193744
C	-4.156990235	1.9226201905	0.7682300967
H	-2.8407360383	0.481384403	1.699211789
C	-4.6186215076	2.4398558133	-0.5990883103
H	-3.8273837926	2.7680051487	1.3878953498
H	-5.0135019786	1.4779542238	1.2908287067
H	-5.4653186721	3.1265634525	-0.4980856467
H	-4.9355300301	1.6116224041	-1.2438295941
H	-3.8208123685	2.9779408296	-1.120981932
C	3.4311509236	0.7510256589	0.5801350409
C	4.7540987859	0.9802994516	-0.1862680864
H	4.8632413315	0.2888744679	-1.0266969101
H	4.8005597127	1.9991136519	-0.5842789964
H	5.612178438	0.833307354	0.4796747696
C	3.3933454539	1.7291373814	1.7687993641
H	4.2728516161	1.5777794518	2.4032695289
H	3.3967190088	2.7709724413	1.432780084
H	2.5080973924	1.5742916906	2.3943505955
C	3.4128478656	-0.6880279014	1.1467416922
H	3.4798985064	-1.437807415	0.3534328861
H	4.2579378221	-0.8452061953	1.8270797589
H	2.4898736211	-0.8725306803	1.7064491903
H	2.4898736211	-0.8725306803	1.7064491903

TS exo 0042

E(RB3LYP) = -706.415425517 A.U.

First frequency = -483.8772 cm^{-1}

H	0.8013809698	-0.4544424732	-3.3680244579
C	0.9415319307	0.1867434723	-2.501934228
H	0.5092121588	1.1750183056	-2.6029859565
C	1.9896818537	-0.0676918274	-1.6346516944
C	2.1480121031	0.6167172131	-0.4074632864
C	1.2658477916	1.6519050855	-0.1273786889
H	1.2827116531	2.1493662873	0.8375532647
H	0.8702856425	2.2629891853	-0.9285636762
C	-0.8036563984	0.7059729243	-0.1409508882
H	-0.5948583383	0.3787452833	0.8749468216
C	-1.645226771	1.955527803	-0.266126472
C	-0.8218441105	-0.2716243807	-1.1330516524
H	-1.4685527485	-0.1042633112	-1.9930050561
C	-0.5099229824	-1.7069741875	-0.7810278639
H	2.5590139949	-0.9752139814	-1.8032929971
H	0.4253278811	-1.7179011363	-0.2097957908
H	-0.3207731517	-2.2928195085	-1.6890891471
C	-1.6209396225	-2.38811217	0.0391092615
H	-1.8117543319	-1.7965162131	0.9446431507
C	-1.2988075967	-3.8373377447	0.4359690697
H	-2.5544606963	-2.3670303524	-0.5386399128
H	-1.1067505913	-4.4279642283	-0.4704168527
H	-2.1857551482	-4.2810188326	0.9060704547
C	-0.1079465497	-3.968606055	1.3936085726
H	-0.2649938924	-3.3676236012	2.2972570994
H	0.8259321675	-3.6310905288	0.932618636
H	0.0383051842	-5.0078199888	1.7057835502
C	-3.1133771526	1.7187905853	0.1306881056
H	-1.6092975009	2.3184405341	-1.3035517613
H	-1.2351471883	2.7616755702	0.3556573449
H	-3.5326594474	0.9287236675	-0.5064835134
C	-3.97962596	2.9790700554	0.0307105961
H	-3.1503184921	1.329470782	1.1579217967
C	-5.4388051837	2.7332041313	0.4250412044

H	-3.9354241432	3.3667173246	-0.9963738872
H	-3.5520520088	3.7638859705	0.6696041512
H	-5.8980676163	1.9747282991	-0.2191754527
H	-6.0377160817	3.6462930618	0.3449106834
H	-5.512200841	2.3751223021	1.4583159964
C	3.1011243455	0.1089954605	0.6958541516
C	4.0882803394	1.2389891282	1.0692263287
H	4.6832303035	1.5369259687	0.1995690926
H	3.5614726593	2.1264958292	1.4318700545
H	4.7756285628	0.9092016458	1.8569906146
C	2.2896511055	-0.2916095428	1.9499406648
H	1.7081528628	0.5457675711	2.3462553682
H	1.5937472639	-1.1059043952	1.7237931185
H	2.9615916966	-0.6329981769	2.7456861957
C	3.9228678709	-1.1155857269	0.2531965118
H	4.609103421	-1.4092860044	1.054172145
H	3.2835814184	-1.9774532638	0.0349527779
H	4.523832036	-0.900400308	-0.6363219084
H	4.523832036	-0.900400308	-0.6363219084

TS exo 0045

E(RB3LYP) = -706.415121598 A.U.

First frequency = -504.9326 cm^{-1}

H	0.9472757066	-1.4466701354	-2.763246915
C	1.04985583	-0.5361753732	-2.1786342197
H	0.5006307008	0.3098992595	-2.5758703829
C	2.1846599476	-0.3543702013	-1.4044521671
C	2.3288735003	0.7247083544	-0.502386339
C	1.313317679	1.6696111995	-0.4627796466
H	1.3131656361	2.4685949455	0.2688371749
H	0.7618249246	1.9028951427	-1.364542962
C	-0.5809569661	0.515632703	0.0543916101
H	-0.259091375	0.5109492662	1.0936962498
C	-1.5885084683	1.5829090391	-0.3112670446
C	-0.5427805481	-0.7017039899	-0.6291543048
H	-1.2645779284	-0.8336947148	-1.4341053216
C	-0.0973449044	-1.9602813234	0.0847952717

H	2.8715014877	-1.1927934761	-1.3179497665
H	0.8338087758	-1.7446821976	0.6202677059
H	0.1463177154	-2.7421791067	-0.6428144754
C	-1.1331063014	-2.4953112222	1.0955610208
H	-0.7099622389	-3.3772838836	1.5970598455
C	-2.4956578587	-2.869717408	0.4913322928
H	-1.2874808969	-1.7370702422	1.874014054
H	-2.9627393562	-1.9722391814	0.0671443578
H	-3.1580764095	-3.2018244186	1.3007691394
C	-2.4244273043	-3.9612538151	-0.5820350977
H	-3.4244307521	-4.2454493683	-0.9256204756
H	-1.9349383098	-4.863051491	-0.1957082153
H	-1.8581746906	-3.6299431391	-1.4588571469
C	-2.983128261	1.3135655099	0.2813319442
H	-1.6735044251	1.6462485899	-1.4058310265
H	-1.2458591999	2.569159411	0.027157263
H	-3.3524106299	0.3503327787	-0.0943541645
C	-4.0010450215	2.4136222923	-0.0390148952
H	-2.8969594606	1.1998797523	1.3711078528
C	-5.3878611588	2.1308239802	0.5457122481
H	-4.0767731649	2.5289114513	-1.1290177534
H	-3.6283395248	3.3741016937	0.3423506072
H	-5.7951192141	1.1910445659	0.1556027326
H	-6.0979998336	2.9283546509	0.3039299991
H	-5.3439610286	2.0420354469	1.6372374175
C	3.4709301936	0.6871672047	0.5334578454
C	3.4922904729	1.9439539899	1.42281568
H	4.346133843	1.9012143852	2.1070285808
H	3.5848541744	2.8572075189	0.8263871367
H	2.5872213502	2.0246819056	2.0337830002
C	3.3280445353	-0.5463746819	1.4553662943
H	2.3859436772	-0.5069081821	2.0122254416
H	3.3441118596	-1.4813607479	0.8883010313
H	4.1484645593	-0.5818780357	2.1815857902
C	4.8204868103	0.6091043591	-0.2167479933
H	5.6529094509	0.5819169285	0.4957961193
H	4.8883903236	-0.2860982068	-0.8414896662
H	4.9545010611	1.4801386708	-0.8662779589

H 4.9545010611 1.4801386708 -0.8662779589

TS exo 0047

E(RB3LYP) = -706.415523883 A.U.

First frequency = -511.7221 cm⁻¹

H 0.7602911031 -0.2129050154 -3.2646527815
C 0.9483585131 0.4087179862 -2.3930560689
H 0.6111692076 1.4334573747 -2.4999630084
C 1.9988557228 0.083903921 -1.5474297971
C 2.2184465843 0.7434611137 -0.3173896635
C 1.3857216015 1.8099861869 -0.0058020341
H 1.4336163921 2.3015627673 0.9585070028
H 1.0062959553 2.4414494091 -0.7990523973
C -0.7307857818 0.9856771979 -0.0323710834
H -0.5459076498 0.5819696997 0.9613604089
C -1.484211913 2.2985259727 -0.0621913204
C -0.8095723955 0.0658992427 -1.0832904335
H -1.4508215181 0.3291578232 -1.9228348176
C -0.6459009301 -1.4114679006 -0.7995741944
H 2.5125732649 -0.857697588 -1.7258346547
H 0.2467272996 -1.5388312144 -0.1797190846
H -0.4549172389 -1.9617071364 -1.7293300573
C -1.8590102934 -2.0375544414 -0.0876990214
H -2.0633229679 -1.4772161497 0.8348879996
C -1.6804559218 -3.5264188818 0.2488997905
H -2.7471995957 -1.9149018617 -0.7216722788
H -1.4653366053 -4.083003227 -0.6737327327
H -2.6325630696 -3.9204033891 0.6267759762
C -0.5806425257 -3.8025834899 1.2815294845
H -0.5356476557 -4.866050075 1.5380926723
H -0.7651103919 -3.243898262 2.2068878774
H 0.4081503121 -3.5111661004 0.9138361936
C -2.9174764059 2.2068368398 0.5042114588
H -1.5290095186 2.6693278462 -1.0963070084
H -0.9423952013 3.0590341791 0.5130851677
H -2.8729027406 1.7887619738 1.5200554707
C -3.894026736 1.3811241644 -0.3394488821

H	-3.3149220067	3.2256953781	0.6127374279
C	-5.3057291885	1.348928343	0.2531415528
H	-3.5156637721	0.3584905523	-0.4394933016
H	-3.9289061	1.7953584878	-1.3568509523
H	-5.7239975617	2.3584760001	0.3394816632
H	-5.2998100231	0.9085599078	1.2569564585
H	-5.9880905581	0.7568327769	-0.3655176986
C	3.2039227521	0.1301428595	0.6986854718
C	4.6020190901	0.0475844991	0.0438369596
H	4.5944331778	-0.5770729352	-0.8540079332
H	4.9544091542	1.0429415005	-0.2452831204
H	5.3275451188	-0.3829547985	0.7436091934
C	3.3251928736	0.979569541	1.9772455114
H	3.6423349756	2.0027642349	1.7518858362
H	2.3777130565	1.0276941724	2.5240170455
H	4.0686261736	0.5375152015	2.6487534128
C	2.7518608202	-1.2899218803	1.1130061843
H	3.4660473821	-1.7311586258	1.8178735741
H	1.7722575477	-1.2601126759	1.6012107723
H	2.6774592265	-1.9600735265	0.2517370894
H	2.6774592265	-1.9600735265	0.2517370894

TS exo 0049

E(RB3LYP) = -706.415408128 A.U.

First frequency = -504.2985 cm^{-1}

H	1.370215045	-0.6162769324	-3.2392341438
C	1.3063726938	0.1475634231	-2.4687501644
H	0.8412977481	1.0703043294	-2.7967195988
C	2.2211243326	0.1354465243	-1.4278712042
C	2.1186309807	0.9961324827	-0.310810293
C	1.0988427354	1.9369558665	-0.3164304814
H	0.9030574555	2.5639293661	0.5451346184
H	0.7710588991	2.3678676672	-1.2537617066
C	-0.8275659014	0.7409739117	-0.5097021705
H	-0.7446862094	0.5114081982	0.5496019372
C	-1.7503689723	1.8840457347	-0.8736149389
C	-0.6017169089	-0.3052906646	-1.4067443304

H	-1.120007245	-0.2495609382	-2.3639919762
C	-0.3044677198	-1.6992893156	-0.900141915
H	2.8906208768	-0.7185660198	-1.3598516924
H	0.4753178381	-1.6383749318	-0.1317448515
H	0.1080092481	-2.3170103609	-1.707477764
C	-1.5374686762	-2.4025541173	-0.307205784
H	-1.9279589352	-1.8024680468	0.5255093368
C	-1.2408597791	-3.8236778863	0.184153946
H	-2.339290197	-2.4335964892	-1.0584642843
H	-0.4331106933	-3.7855262457	0.9279942858
H	-0.8546173732	-4.422753625	-0.6518150528
C	-2.4660729237	-4.514502136	0.7895673191
H	-2.8516091132	-3.9510475245	1.6470495622
H	-2.2301514746	-5.5267125979	1.1341268562
H	-3.2767632826	-4.5917486199	0.0559814527
C	-3.2470007623	1.5366234107	-0.7217359342
H	-1.5672350495	2.1741771934	-1.9173616265
H	-1.5219569962	2.7692615711	-0.2691199469
H	-3.8408445395	2.4099091141	-1.0265320428
C	-3.6715022504	1.1117059275	0.6930482673
H	-3.4920886222	0.7288928153	-1.4230009361
C	-3.3854372323	2.1602343366	1.7734945587
H	-3.1700787056	0.1723155164	0.9558297119
H	-4.7456257268	0.8877883105	0.681095156
H	-3.7811585092	1.8460389499	2.744734167
H	-3.8444926474	3.1234237186	1.5212915299
H	-2.3105881324	2.3303124784	1.8971554384
C	2.9767274821	0.7078442545	0.9379263033
C	2.6436186948	-0.6883440894	1.5140772657
H	3.2619873371	-0.8998153336	2.394218934
H	1.5931473499	-0.7412864729	1.8191027961
H	2.8213171798	-1.4822292406	0.7832103571
C	4.4693827145	0.7513727366	0.5379545778
H	4.7080149258	0.0078516195	-0.2279065743
H	4.7363790987	1.7362570103	0.141403712
H	5.1044221525	0.5488379695	1.4080568832
C	2.7511563741	1.7466771325	2.0519515819
H	3.4150140132	1.5363837337	2.8969891132

H	2.9623715271	2.7626077144	1.7032679099
H	1.7235211715	1.7213196819	2.4292621177
H	1.7235211715	1.7213196819	2.4292621177

TS exo 0055

E(RB3LYP) = -706.416099516 A.U.

First frequency = -501.0026 cm⁻¹

H	1.4946363604	-0.929358257	-3.0792742294
C	1.3903492111	-0.0992393154	-2.385654778
H	0.8264016173	0.7392656771	-2.7782792819
C	2.341598995	0.0767149644	-1.3938820921
C	2.2030027252	1.033821389	-0.3619667693
C	1.1024934756	1.8777260027	-0.4117619601
H	0.8853576112	2.5714609402	0.3914710657
H	0.7046152675	2.1818979294	-1.3712944491
C	-0.7165046738	0.5140241445	-0.3982196752
H	-0.5831456523	0.4069082399	0.6752040997
C	-1.7417059368	1.5367783609	-0.8410901649
C	-0.432065996	-0.6006888185	-1.1893546246
H	-0.9803798238	-0.6867917682	-2.1260101294
C	0.0175052824	-1.899851084	-0.5514705887
H	3.0917310454	-0.7015111221	-1.2760136956
H	0.8895114026	-1.6951686642	0.0792767663
H	0.3542130015	-2.5982714879	-1.3277498669
C	-1.0632924956	-2.580492485	0.3113713828
H	-0.6347872074	-3.4802104795	0.7750802383
C	-2.3316078956	-2.9668525106	-0.4568334665
H	-1.3337084079	-1.9107859198	1.1390585563
H	-2.0642516923	-3.6497254713	-1.2752039971
H	-2.7539575253	-2.0725043231	-0.9308246862
C	-3.3924509442	-3.6149881785	0.436595766
H	-3.007220543	-4.5225309863	0.9156415912
H	-4.2862101652	-3.8910967957	-0.1325372674
H	-3.7034746078	-2.9284597899	1.2326200811
C	-3.201831562	1.0528134127	-0.7025608883
H	-1.5655291725	1.7922787379	-1.8951472769
H	-1.6126420676	2.4683506894	-0.2783980643

H	-3.8703227406	1.8662999754	-1.0178751584
C	-3.6004219361	0.590764491	0.7074127586
H	-3.3651160018	0.2257772516	-1.4050290008
C	-3.4239196437	1.6624076462	1.7882669379
H	-3.0145048974	-0.2965309604	0.9749075904
H	-4.6484069413	0.2662608785	0.6848912018
H	-3.9748962991	2.5754807031	1.5338825722
H	-2.371391149	1.9376348851	1.9147689207
H	-3.7898749239	1.3109222799	2.7583681703
C	3.1363201199	0.955435062	0.8632834048
C	2.9752102179	-0.4035191001	1.5840139205
H	1.9484810814	-0.5333786256	1.9419563013
H	3.2096710762	-1.2435972443	0.9242131123
H	3.6451869128	-0.4623294755	2.4496697597
C	4.5984091546	1.1080806524	0.3846074718
H	4.7449000969	2.0713075245	-0.1146633002
H	5.2869658958	1.0552680189	1.235789054
H	4.8801553193	0.3208508299	-0.3205479466
C	2.8501270194	2.0706395052	1.8857782836
H	3.5646225846	2.0089281874	2.7132118763
H	2.943442215	3.0637788676	1.4349406258
H	1.8458967748	1.9819273396	2.3132674676
H	1.8458967748	1.9819273396	2.3132674676

TS exo 0058

E(RB3LYP) = -706.415904423 A.U.

First frequency = -501.4214 cm⁻¹

H	1.1804786632	-1.4532078313	-2.7614184925
C	1.234341518	-0.5189737831	-2.2086509029
H	0.750272293	0.3165898429	-2.7017646209
C	2.2773215217	-0.3200081429	-1.3182812114
C	2.3415445287	0.7964581195	-0.4526486583
C	1.3538107459	1.7633068869	-0.5752848895
H	1.2887122028	2.596006457	0.1145646171
H	0.9191264416	1.96461495	-1.5456942872
C	-0.6198715456	0.6694174325	-0.2386749452
H	-0.4176312104	0.7185743086	0.8277429702

C	-1.541085952	1.7359597889	-0.7956341535
C	-0.5297217037	-0.5841233669	-0.8465810762
H	-1.1564310001	-0.7492172906	-1.7219555074
C	-0.1923890132	-1.8107572201	-0.0250619689
H	2.9327574755	-1.1641895368	-1.1184306515
H	0.7205250933	-1.6088249487	0.5457104795
H	0.0439512853	-2.6502761215	-0.6883145422
C	-1.3017347638	-2.225913093	0.9647064248
H	-0.9684174097	-3.1229045414	1.5056236649
C	-2.672552914	-2.5025308978	0.3286808787
H	-1.4149146652	-1.4353925604	1.7177448378
H	-3.052142622	-1.5788177052	-0.1243049605
H	-3.3821306158	-2.7639469226	1.1240351225
C	-2.6582927101	-3.6162500293	-0.7235683657
H	-2.0386347064	-3.3480211702	-1.5858146178
H	-3.6668910692	-3.823528489	-1.095760285
H	-2.2574539008	-4.5479557276	-0.3073245797
C	-3.0380996354	1.4467421967	-0.5633357093
H	-1.3721000658	1.8293858691	-1.8775978377
H	-1.2925762627	2.7120325143	-0.3602399897
H	-3.6326806918	2.2424711288	-1.0337223957
C	-3.4335502406	1.329528381	0.9125099529
H	-3.3045037648	0.5166094088	-1.08289419
C	-4.9218914749	1.0257646318	1.1032037888
H	-3.1727063966	2.2619860726	1.4321103948
H	-2.8392124306	0.5385148039	1.3852537185
H	-5.5472897919	1.8063874825	0.6548966467
H	-5.1860429518	0.9535213351	2.1632929555
H	-5.1891139329	0.0749042982	0.6278117388
C	3.3557008927	0.7858320986	0.7093316454
C	4.7809330071	0.6595461432	0.1235979865
H	5.5253820703	0.6499839054	0.9280223339
H	4.9038210252	-0.2610373444	-0.4541208084
H	5.004286344	1.5017550384	-0.5392187207
C	3.2967215786	2.077275487	1.5457615838
H	2.3280264055	2.1956081245	2.0423499661
H	4.0637109396	2.0500311085	2.326771334
H	3.4759509158	2.964254273	0.9297873944

C	3.0862955653	-0.4070125578	1.6561279613
H	3.8149949599	-0.4211172273	2.4749694713
H	2.0858889278	-0.3349320805	2.0956442041
H	3.1551668494	-1.3648289906	1.1327917362
H	3.1551668494	-1.3648289906	1.1327917362

TS exo 0064

E(RB3LYP) = -706.415676366 A.U.

First frequency = -483.0893 cm⁻¹

H	1.1052690188	-0.5140042419	-3.3902225687
C	1.1829496593	0.1733174495	-2.5520984971
H	0.8163753765	1.1719603157	-2.7581527247
C	2.1169063202	-0.0725001933	-1.5605383218
C	2.1767946327	0.6805776504	-0.3651972754
C	1.3264756417	1.7716952003	-0.2461151672
H	1.2640991189	2.3278903428	0.6842127999
H	1.0521221908	2.3475064151	-1.120591369
C	-0.7781011565	0.9169047583	-0.4383897591
H	-0.6880494605	0.6458394204	0.609595325
C	-1.528208331	2.1969232695	-0.7379972116
C	-0.7381517003	-0.119435037	-1.3682264464
H	-1.2786982804	0.0216461163	-2.3029832854
C	-0.5423730449	-1.5426705001	-0.9015698533
H	2.653765738	-1.0133837489	-1.6119973587
H	0.3261511005	-1.5620058235	-0.2334937551
H	-0.2917983473	-2.1932051837	-1.7487420435
C	-1.7678691525	-2.117273487	-0.1673077726
H	-2.0112945566	-1.4685969874	0.6850694445
C	-1.5736827104	-3.5576918092	0.3312581593
H	-2.6370127211	-2.0764984371	-0.8370380264
H	-1.3295066724	-4.2069914775	-0.5208016951
H	-2.5274478411	-3.9254108277	0.730764553
C	-0.4923888575	-3.7003110891	1.4096032447
H	0.5008468839	-3.441731959	1.0286687748
H	-0.4408724237	-4.7266464593	1.7874156437
H	-0.7002990592	-3.0412826603	2.2610327607
C	-3.0578642014	2.0555129436	-0.5997303482

H	-1.2960237795	2.5167143629	-1.763325729
H	-1.1846156064	3.0035623742	-0.0778105275
H	-3.533689589	2.9925997142	-0.9214066691
C	-3.5266247956	1.718533527	0.8204161183
H	-3.4067473366	1.2753583535	-1.2896220891
C	-5.0503055331	1.6185948589	0.9332576232
H	-3.1525439955	2.4835905422	1.5150805388
H	-3.0754303638	0.7702426148	1.1373986523
H	-5.4418091317	0.8379475099	0.2709221545
H	-5.5308384809	2.5621370694	0.6498623201
H	-5.3641299241	1.3775705489	1.954197144
C	2.9754324951	0.2001153959	0.8655070359
C	2.0109991381	-0.0851281431	2.0404879114
H	2.5726725217	-0.4064851625	2.925075131
H	1.4335520999	0.800594594	2.3204886254
H	1.3029833197	-0.8797703959	1.7837614261
C	3.7768016819	-1.085212	0.5885110552
H	4.355042664	-1.3588975317	1.4770261536
H	3.1220544872	-1.9296673419	0.3490365788
H	4.482003304	-0.9527389489	-0.2384462847
C	3.9724607041	1.3054337466	1.2837128236
H	4.6741034014	1.5220195018	0.4714281861
H	3.4555550441	2.2364327153	1.5341199086
H	4.5509583084	0.9941940149	2.1613293166
H	4.5509583084	0.9941940149	2.1613293166

TS exo 0066

E(RB3LYP) = -706.414618560 A.U.

First frequency = -503.1102 cm^{-1}

H	0.9944322441	-0.2514812988	-3.2907164568
C	1.002321507	0.3605044933	-2.3925967301
H	0.4936128866	1.311772609	-2.4997463749
C	2.0204424629	0.190550743	-1.4682284204
C	2.0242574621	0.8335280602	-0.2088346408
C	0.9997749095	1.7306570657	0.0577129613
H	0.8877798722	2.187708899	1.0335269328
H	0.5717770632	2.3122179341	-0.7488490886

C	-0.9283285587	0.5373654496	-0.1580511738
H	-0.7443319836	0.1321418041	0.8346574149
C	-1.9043837074	1.6907645591	-0.220964414
C	-0.7769431156	-0.3335067715	-1.2387725299
H	-1.3915678135	-0.1388150388	-2.1174567511
C	-0.3968285225	-1.7769423462	-0.9968828536
H	2.7035463063	-0.6410320895	-1.6234393081
H	0.4596815129	-1.7943094872	-0.3158524968
H	-0.0587628859	-2.2471764794	-1.9288714937
C	-1.5478050023	-2.6084245219	-0.4016534972
H	-1.8791367773	-2.1407695812	0.5354819737
C	-1.1819372148	-4.077419843	-0.1384802323
H	-2.408199629	-2.5639518862	-1.0827815067
H	-0.8483235619	-4.5414932506	-1.0769447372
H	-2.0871751556	-4.6193925933	0.1638886725
C	-0.1041869747	-4.2656103334	0.9363628803
H	0.8506486344	-3.8204404632	0.6395426434
H	0.0758976188	-5.3269328264	1.1364193938
H	-0.4070186013	-3.7951323596	1.8794276782
C	-3.3547210115	1.2426614391	0.0437046558
H	-1.854408819	2.1592688764	-1.214943365
H	-1.6231279861	2.4663710127	0.5000791063
H	-3.6099687229	0.454975768	-0.6760950519
C	-4.3918055345	2.3729013361	-0.0456615866
H	-3.4089031523	0.7754422443	1.037314833
C	-4.2402053643	3.4524274926	1.0323917678
H	-5.3954021343	1.934622265	0.0267174632
H	-4.3336115758	2.8371053877	-1.0399559519
H	-3.2892393615	3.9871806117	0.943155668
H	-4.2788601655	3.011652378	2.0355002609
H	-5.0413188556	4.1956067557	0.9638912269
C	3.0139273656	0.354443815	0.8731039469
C	2.7707559207	-1.1347721787	1.2139378203
H	2.882019284	-1.7760521619	0.3348658874
H	3.4859299829	-1.4786912003	1.9701462172
H	1.7617747253	-1.2833339314	1.6124896489
C	4.4546577113	0.5255197867	0.3390817628
H	5.1823712483	0.1934246317	1.088458966

H	4.6239678007	-0.0581032769	-0.5703545487
H	4.6595355072	1.5751202498	0.1047725634
C	2.8891055083	1.1647441905	2.1764109794
H	1.9067580703	1.0353845529	2.642477192
H	3.6406566999	0.8275472886	2.8978618134
H	3.0467698034	2.2338484817	2.0018932512
H	3.0467698034	2.2338484817	2.0018932512

TS exo 0068

E(RB3LYP) = -706.415590958 A.U.

First frequency = -489.9941 cm^{-1}

H	0.7828247537	0.0549065245	-3.3514594532
C	0.9603728944	0.5982312653	-2.4271554654
H	0.5974111492	1.6189410872	-2.4334307393
C	1.9902124325	0.1941390793	-1.5935234307
C	2.1859910998	0.7418191093	-0.3057276604
C	1.365147147	1.7956695481	0.0760922715
H	1.407506475	2.194416267	1.0851363785
H	1.0165901084	2.5072509114	-0.6614504841
C	-0.7567430315	0.9964378159	-0.0249963505
H	-0.5741538512	0.5561493782	0.9531643903
C	-1.5167179954	2.305242371	-0.009415946
C	-0.8225348202	0.1210439251	-1.1094868417
H	-1.4548595752	0.4044627472	-1.948187142
C	-0.5901036855	-1.35666044	-0.8934075242
H	2.5009536914	-0.7269510374	-1.8523343893
H	0.3395675448	-1.4696822578	-0.3244346668
H	-0.4248529874	-1.8628644564	-1.8524731451
C	-1.7365529854	-2.0592328886	-0.1430191124
H	-1.9176915065	-1.537809764	0.8066156609
C	-1.4739728402	-3.54758118	0.1360805503
H	-2.6609062621	-1.9579579962	-0.7269349698
H	-1.2898215635	-4.068038367	-0.8138646275
H	-2.3840838192	-3.9942614508	0.5563501295
C	-0.3041913084	-3.8033727278	1.094573339
H	-0.2028775908	-4.8696549917	1.3215787834
H	-0.4524045827	-3.2729301458	2.0427673225

H	0.6492522117	-3.46650309	0.6750392448
C	-2.9462928498	2.1823380856	0.5600367543
H	-1.5684896635	2.7088919707	-1.0307224094
H	-0.9775112188	3.050069903	0.588510825
H	-2.8913384015	1.7502902759	1.569513766
C	-3.9108930741	1.3512048832	-0.2921953517
H	-3.3603106258	3.1926922952	0.684419678
C	-5.3212437359	1.2905649862	0.3013557484
H	-3.5160287184	0.3357042368	-0.4044387332
H	-3.9532990697	1.7760404873	-1.3049363216
H	-5.3072719698	0.8406202261	1.3008403924
H	-5.9947442567	0.693756414	-0.3224554641
H	-5.7554847513	2.2924073436	0.3979512399
C	3.1041943281	0.073200324	0.7394359561
C	3.8427634906	-1.1566524166	0.1801927892
H	3.1473485648	-1.949739402	-0.1141886116
H	4.4575066188	-0.8998693221	-0.6886200465
H	4.5072772641	-1.568907792	0.9464707588
C	4.1636835248	1.0976709938	1.2071786095
H	4.7761367182	1.4342229534	0.3641623999
H	3.6958512342	1.9808083413	1.652140439
H	4.8285913925	0.6535857771	1.9571581985
C	2.2704296114	-0.3870213401	1.9579555891
H	2.9202381912	-0.8431651836	2.7135394298
H	1.7461687788	0.446348811	2.4343395835
H	1.5221012171	-1.1300137923	1.6641191113
H	1.5221012171	-1.1300137923	1.6641191113

TS exo 0081

E(RB3LYP) = -706.415593890 A.U.

First frequency = -520.5752 cm⁻¹

H	1.3674538955	-0.48412984	-3.3777011511
C	1.3406119083	0.1912715655	-2.5263801823
H	0.8889701935	1.15334789	-2.7415384232
C	2.2954304598	0.0557153156	-1.5282485053
C	2.2439166484	0.7928258895	-0.3251277478
C	1.2368745702	1.7406884685	-0.1995086251

H	1.0744313277	2.2729852578	0.7301431724
H	0.8972557409	2.2793240033	-1.0750407624
C	-0.7072957422	0.604506406	-0.471344935
H	-0.607232743	0.2864855696	0.5615142938
C	-1.6152708128	1.792075984	-0.7222579109
C	-0.5146809248	-0.3643036598	-1.4638885099
H	-1.063888691	-0.2197200321	-2.3952970051
C	-0.2130600957	-1.8083658804	-1.1147267831
H	2.9506425004	-0.8106321297	-1.5759895613
H	0.4317631411	-1.8333711208	-0.2304327855
H	0.3676679775	-2.2724236566	-1.9197600878
C	-1.465166222	-2.6825528327	-0.8824312433
H	-2.0800049771	-2.6590974405	-1.7925991573
C	-2.3449421726	-2.3054996433	0.3179603473
H	-1.1347095835	-3.7243885727	-0.7653298999
H	-3.2211723873	-2.9665116816	0.3266538459
H	-2.7309765153	-1.2912485986	0.1794072965
C	-1.6362116867	-2.4015438554	1.6728362637
H	-0.800627502	-1.697948969	1.7463163345
H	-1.2314977353	-3.4071456359	1.8366898561
H	-2.3243191125	-2.1797061117	2.4952699124
C	-3.1054302592	1.5004132327	-0.4516113899
H	-1.4976019568	2.1090398395	-1.7674942163
H	-1.3134629259	2.6488345814	-0.1059098954
H	-3.711842966	2.3302592352	-0.840290589
C	-3.4346565951	1.3052284957	1.0340917557
H	-3.4046707432	0.6085970051	-1.0183553992
C	-4.8934198653	0.9060609267	1.2706074341
H	-3.2093688081	2.2352913602	1.5735574346
H	-2.7772033808	0.5399998154	1.4640239059
H	-5.1188556406	-0.049982177	0.7841776231
H	-5.5808060661	1.6550758618	0.8608479995
H	-5.1141873478	0.7976510975	2.3374902589
C	3.1299096404	0.3591608481	0.8602621227
C	4.6103766835	0.3894682405	0.4167576377
H	5.262923406	0.0867930808	1.2437243265
H	4.8000056106	-0.2882046083	-0.4204566515
H	4.9010075543	1.3972040424	0.1028530992

C	2.9773534641	1.2949154169	2.07370179
H	3.6625640383	0.9866128983	2.8702576966
H	3.2092775245	2.3323857149	1.8125406688
H	1.9633159442	1.2647060832	2.4856428911
C	2.761701366	-1.0731368409	1.3128792525
H	1.7229388661	-1.1158254261	1.657438068
H	2.8755767175	-1.7969620335	0.5010925773
H	3.404234675	-1.3935074955	2.1412660999
H	3.404234675	-1.3935074955	2.1412660999

TS exo 0083

E(RB3LYP) = -706.416152690 A.U.

First frequency = -478.0771 cm^{-1}

H	1.4127717111	-1.1558115592	-3.1318403183
C	1.363568252	-0.2981808957	-2.4664813706
H	0.8140961784	0.5464373589	-2.8646597942
C	2.3273656069	-0.1453927065	-1.4858833114
C	2.2490723891	0.8519336142	-0.4857399487
C	1.2071461534	1.765895902	-0.564081118
H	1.0462108558	2.4926787588	0.2263021329
H	0.8234453957	2.0741195517	-1.5279470913
C	-0.6966032292	0.5223046211	-0.4644072695
H	-0.5519390317	0.4911157508	0.6121048615
C	-1.6680242079	1.5655511566	-0.9734567426
C	-0.4828272731	-0.6598914621	-1.1682343112
H	-1.03714982	-0.7953097637	-2.0947286578
C	-0.0482420121	-1.9145677631	-0.4412946206
H	3.0326750011	-0.9590805552	-1.3566051845
H	0.8603600448	-1.6879561345	0.1306232565
H	0.2293144337	-2.6893766498	-1.1665560811
C	-1.1112721755	-2.4746921033	0.5245905911
H	-0.695230387	-3.3471400387	1.047856355
C	-2.4259523071	-2.8740851616	-0.1539568825
H	-1.320142047	-1.7249838744	1.2998193094
H	-2.2211431128	-3.6372765383	-0.9175524443
H	-2.8332041035	-2.0076647504	-0.6894364134
C	-3.4706854468	-3.3953191408	0.8361989396

H	-4.3982698911	-3.6831802084	0.3305818763
H	-3.7203684623	-2.6284632941	1.5787310136
H	-3.099842332	-4.2720801008	1.3795967069
C	-3.1490098021	1.1767700617	-0.7705071056
H	-1.4988925776	1.7260663287	-2.047109199
H	-1.4751376151	2.5293449639	-0.4886424245
H	-3.7799028557	2.0001225743	-1.1338285712
C	-3.5376568294	0.8446959723	0.6786131626
H	-3.3731173626	0.3089997413	-1.4037715053
C	-3.2694913169	1.9796310265	1.6725265212
H	-2.9990241025	-0.0550127789	0.9992604977
H	-4.6033563541	0.5844349804	0.7028475715
H	-3.6318327701	1.7236917694	2.6733941713
H	-3.7699796375	2.9043142104	1.361948578
H	-2.1993018347	2.1968637258	1.7568827282
C	3.1302738695	0.8120892609	0.7808143823
C	3.8840724048	2.1551980139	0.9171668874
H	4.5132797524	2.1566733019	1.8147991237
H	4.5280014077	2.3281974255	0.0486007009
H	3.1911919424	2.9984073499	0.9909899254
C	2.2416748838	0.5984516443	2.0282579055
H	2.8548624181	0.5818419918	2.9365555691
H	1.501469183	1.3954967406	2.1441782056
H	1.7025943653	-0.3524877406	1.9655121767
C	4.1752864859	-0.3180163025	0.7416876883
H	4.8347218207	-0.2290632023	-0.1277988987
H	4.8011793809	-0.2737858721	1.638942025
H	3.7057916318	-1.3067624181	0.7166131716
H	3.7057916318	-1.3067624181	0.7166131716

TS exo 0084

E(RB3LYP) = -706.415901842 A.U.

First frequency = -478.3251 cm^{-1}

H	1.1220387497	-1.5433997779	-2.8313737542
C	1.211646018	-0.6097102513	-2.2827301318
H	0.7271273294	0.2357141248	-2.7568011625
C	2.2575277618	-0.4458715928	-1.3917716617

C	2.3590108324	0.6708416282	-0.5295181628
C	1.4154535059	1.6799705715	-0.6636883645
H	1.3907773034	2.5127522768	0.0324109239
H	0.9925450857	1.9061372028	-1.633693669
C	-0.6025797506	0.6739946547	-0.2944458999
H	-0.3842234955	0.7652457379	0.7657098065
C	-1.4936022068	1.7441822928	-0.8906406281
C	-0.5556565598	-0.6036849685	-0.8454464034
H	-1.1874790491	-0.7975871308	-1.710384972
C	-0.1989980203	-1.7944590422	0.0163047904
H	2.8816905068	-1.3117064157	-1.1995720212
H	0.7452941834	-1.5808110058	0.5324127759
H	-0.0073973298	-2.6690975988	-0.6149290613
C	-1.2669119085	-2.1377979921	1.0769658514
H	-0.9260756745	-3.0143134237	1.6459941869
C	-2.6709596094	-2.414357514	0.5178643451
H	-1.3295547122	-1.3087964682	1.7936028878
H	-3.0508972878	-1.5054722101	0.035657561
H	-3.3486237405	-2.6194343211	1.3563799018
C	-2.727997398	-3.5790680566	-0.4761175036
H	-3.7566634985	-3.7811626841	-0.7919517118
H	-2.3281153629	-4.4979851175	-0.0314846966
H	-2.1430079717	-3.3682917086	-1.3776134136
C	-2.9951195449	1.5124855642	-0.62483858
H	-1.3358713459	1.7819233504	-1.9775727727
H	-1.2080753628	2.7303962453	-0.503455662
H	-3.5734283734	2.3021808411	-1.1246621782
C	-3.3707318536	1.4777161565	0.8606091775
H	-3.2961241663	0.5664508049	-1.0946195287
C	-4.8645775755	1.2305526322	1.0867713811
H	-3.0731629621	2.4250172264	1.3313354063
H	-2.7938492282	0.6915091847	1.3623566348
H	-5.4725421024	2.0086124043	0.6108839703
H	-5.1140251455	1.2166485415	2.1527705394
H	-5.1687149651	0.267337603	0.6609752078
C	3.3281388558	0.6915409689	0.6717430492
C	4.2296885561	1.9439292226	0.5735653827
H	4.9251703622	1.9878097711	1.4197823179

H	4.8169435369	1.9273548228	-0.3504717377
H	3.6387492022	2.8644423801	0.5758553705
C	2.5244068534	0.7458257336	1.9916105904
H	3.2031299496	0.774989531	2.8517077243
H	1.8855838633	1.6321060654	2.0449932333
H	1.8834050679	-0.1357764639	2.0954359215
C	4.2398458148	-0.5482938408	0.720563367
H	3.6665823236	-1.4706569379	0.8595485939
H	4.8353581507	-0.6486718209	-0.192696789
H	4.9348889194	-0.4628987741	1.5622313541
H	4.9348889194	-0.4628987741	1.5622313541

TS exo 0088

E(RB3LYP) = -706.413984219 A.U.

First frequency = -502.1631 cm^{-1}

H	0.5414223947	-0.8258528996	-3.0526505724
C	0.7181825042	-0.056075621	-2.3060691371
H	0.2289782609	0.8878455631	-2.5178204113
C	1.8698356494	-0.1108854696	-1.5379997334
C	2.1040840844	0.7598627252	-0.4486912438
C	1.1646118921	1.7512265399	-0.2047213605
H	1.2315603896	2.3917604745	0.6663766564
H	0.6222584918	2.1927979304	-1.0310021746
C	-0.8029505108	0.6540617017	0.1319155148
H	-0.4664532112	0.4231810587	1.1405718082
C	-1.7399767043	1.8347126209	0.0096841911
C	-0.8681362899	-0.4051495482	-0.7751926031
H	-1.6124276023	-0.3267907522	-1.5675823593
C	-0.520233572	-1.8097503922	-0.3343366376
H	2.4912187156	-0.9983592274	-1.6304653463
H	0.4238483182	-1.7820963603	0.2234615558
H	-0.3425574212	-2.4437948989	-1.2094041811
C	-1.6078799198	-2.4394181549	0.5559970671
H	-1.7988028409	-1.7664191653	1.4014099804
C	-1.2496735928	-3.8349152658	1.0902869523
H	-2.5508832811	-2.4940431643	-0.0066988165
H	-2.0193238132	-4.1458557607	1.8084114417

H	-0.3109662811	-3.7708676474	1.6580415832
C	-1.1169963108	-4.9093458259	0.0048160765
H	-0.2937253901	-4.6928604694	-0.6833146908
H	-2.0352947759	-4.9800554056	-0.5900240009
H	-0.9273541666	-5.8945502858	0.4433929158
C	-3.1314957971	1.535088725	0.5997126704
H	-1.8392891819	2.104664289	-1.049996178
H	-1.3247167548	2.7162339499	0.5154727467
H	-3.572992349	0.6894362823	0.0553114851
C	-4.0983028229	2.7287346134	0.5744502324
H	-3.0047509762	1.1953712993	1.6362955654
C	-4.4767001835	3.1958554344	-0.8358415875
H	-3.6536860378	3.5655728296	1.1306504525
H	-5.0114843461	2.4536492723	1.1175186398
H	-3.6087064478	3.5727456054	-1.386249725
H	-5.2175653806	4.0012365672	-0.8012850088
H	-4.9057405933	2.372279462	-1.4186830891
C	3.2454127825	0.4349264638	0.536366935
C	3.3710428454	1.4899747497	1.6509190534
H	2.479036063	1.5192725229	2.2852846603
H	4.2231832196	1.2507049936	2.29562355
H	3.5313075592	2.4918265311	1.2398931715
C	3.0094769764	-0.9393756662	1.2057223065
H	3.8278124414	-1.1780551984	1.8950083855
H	2.0759646944	-0.9364267626	1.7782599949
H	2.9484426295	-1.7451104419	0.4688008414
C	4.5807372366	0.4002948956	-0.2418857795
H	5.4118484253	0.1709026804	0.434891668
H	4.5741568034	-0.358808894	-1.0292721268
H	4.7804792834	1.3680435276	-0.7131690165
H	4.7804792834	1.3680435276	-0.7131690165

TS exo 0098

E(RB3LYP) = -706.415286198 A.U.

First frequency = -506.0105 cm^{-1}

H	1.2053153659	-0.6890414461	-3.2846402763
C	1.1902237739	0.0605781165	-2.4978191028

H	0.7965106993	1.0216122565	-2.8088061739
C	2.0929994684	-0.0410680503	-1.4510313863
C	2.0430219592	0.7993879868	-0.3152364803
C	1.0981443923	1.8159249598	-0.3100560773
H	0.9400833851	2.4369336206	0.5635205715
H	0.8180771951	2.2923764753	-1.2408616118
C	-0.9129822359	0.7818170225	-0.5543330287
H	-0.8657691287	0.5400199443	0.5042998083
C	-1.7389258155	1.9944930064	-0.924343273
C	-0.7516209147	-0.2731911663	-1.4552970223
H	-1.2560481615	-0.1801343009	-2.4168936342
C	-0.543822907	-1.6818359176	-0.9457905917
H	2.6977353411	-0.9431494246	-1.3975657425
H	0.2440006514	-1.6574830247	-0.1867924536
H	-0.1751725844	-2.3293313136	-1.7513966706
C	-1.8181192766	-2.3032748772	-0.3457633927
H	-2.168973204	-1.671582431	0.4814336771
C	-1.6285195907	-3.7417183523	0.1601347777
H	-2.6149289623	-2.2842373989	-1.1011690791
H	-1.2747070412	-4.3728153072	-0.6668305616
H	-2.6056974897	-4.145404361	0.454622234
C	-0.6611072127	-3.8601098536	1.3442709384
H	-0.6092157566	-4.8896970493	1.7131426277
H	-0.9835459204	-3.2234127336	2.1768074628
H	0.3549231803	-3.5562538796	1.0735154781
C	-3.260259486	1.7620813984	-0.8006886548
H	-1.515631286	2.2773900762	-1.9622769154
H	-1.4537519423	2.8549566173	-0.3082862822
H	-3.7799131853	2.6812027346	-1.1061772067
C	-3.7401290036	1.3580992579	0.6024525239
H	-3.5545801105	0.9819897312	-1.5141903477
C	-3.3912973628	2.3707074062	1.6986050028
H	-3.317755325	0.3799185282	0.8627738938
H	-4.8280971151	1.2189169527	0.5710183946
H	-3.769671164	3.3691659409	1.449616298
H	-2.3086688845	2.4551920922	1.8410770044
H	-3.8263665084	2.0790821734	2.65999968
C	2.8667636049	0.4222431882	0.9332800494

C	4.3628538777	0.3785801124	0.5460879194
H	4.6967696478	1.353688557	0.1770614293
H	4.9754643126	0.1131145682	1.4153712008
H	4.5592295972	-0.359251442	-0.2371180606
C	2.6981612517	1.4444329923	2.0724187724
H	3.3355505163	1.1673509313	2.9185534456
H	2.982182273	2.4524222991	1.753728135
H	1.6663604295	1.4790853668	2.4374599296
C	2.4395461991	-0.9636508035	1.4714900277
H	2.5701329613	-1.7487186659	0.7211857813
H	3.0378369947	-1.2375965742	2.3481736579
H	1.3864337508	-0.957341529	1.7712420756
H	1.3864337508	-0.957341529	1.7712420756

TS exo 0108

E(RB3LYP) = -706.415512674 A.U.

First frequency = -521.5358 cm⁻¹

H	0.8005071057	-0.5751582491	-3.0599182687
C	0.9515106471	0.1728581865	-2.285764737
H	0.4439444067	1.1118017501	-2.4754952716
C	2.1113650095	0.1284403934	-1.5240515702
C	2.3174104923	0.9644996152	-0.4051644726
C	1.3378104264	1.9090398161	-0.1267764884
H	1.3778181171	2.5189322404	0.7679181344
H	0.7924721812	2.3662460178	-0.9423392315
C	-0.6006291234	0.7627054851	0.1501725935
H	-0.2721194455	0.5182606209	1.1589249933
C	-1.5693070547	1.9250456671	0.0520911659
C	-0.6008974892	-0.2799384439	-0.7855862948
H	-1.3394630957	-0.2226779567	-1.5826015835
C	-0.1696085757	-1.673575219	-0.3705325661
H	2.7609226063	-0.7344651984	-1.6496288306
H	0.7477780959	-1.5854927215	0.2210726388
H	0.091363567	-2.2683730232	-1.2545663631
C	-1.2266405035	-2.4380296017	0.4494468912
H	-0.7744594709	-3.3548439488	0.8529080619
C	-2.4772807011	-2.8166512206	-0.3538171143

H	-1.5150287942	-1.8317195252	1.3187533042
H	-2.1845778929	-3.4884367669	-1.1723245059
H	-2.8952483175	-1.9226729775	-0.8314619109
C	-3.5572302004	-3.4812018342	0.5036642695
H	-3.1763683109	-4.3870216341	0.9893882817
H	-4.4301348076	-3.7639904174	-0.0938522802
H	-3.8995176752	-2.80270829	1.2936745462
C	-2.8078566916	1.7858048173	0.9649745219
H	-1.8844806593	2.0462731705	-0.9924466775
H	-1.0756106985	2.8654296351	0.3268564271
H	-2.4618857522	1.7298744303	2.006069004
C	-3.722934426	0.5861757069	0.6836355544
H	-3.3960778101	2.7110117117	0.888290777
C	-4.3671636062	0.5984165214	-0.7057832011
H	-4.5137214998	0.5672656173	1.4444819007
H	-3.1534800996	-0.3392523979	0.8125659113
H	-4.9397794198	1.5191031644	-0.8683927899
H	-5.0507676895	-0.2476983061	-0.8307561955
H	-3.6171628765	0.5327322853	-1.5003859972
C	3.478952393	0.6567630293	0.5616814673
C	4.8076190093	0.7140820051	-0.2267830109
H	5.6548206678	0.5020786268	0.4355784288
H	4.8300945133	-0.0169309626	-1.0400924789
H	4.9561769871	1.7060029552	-0.6655737064
C	3.5629503386	1.6761724779	1.7126174583
H	3.6751071785	2.6983295979	1.3372132116
H	2.6739963514	1.6420308469	2.3510483641
H	4.4287254618	1.4532899783	2.3449196448
C	3.3157063106	-0.7501024282	1.1823842667
H	4.154262094	-0.9755734033	1.8515046718
H	2.3921291945	-0.810951407	1.7675819386
H	3.2807043228	-1.5304798416	0.4170152575
H	3.2807043228	-1.5304798416	0.4170152575

TS exo 0112

E(RB3LYP) = -706.415603734 A.U.

First frequency = -500.2161 cm^{-1}

H	0.807150579	-0.3044645165	-3.1884191519
C	0.955329362	0.372861207	-2.351481369
H	0.4253862637	1.3134701182	-2.4417983207
C	2.1045335085	0.2560493145	-1.5848029564
C	2.2994928454	0.9885384235	-0.39333715
C	1.3265751219	1.91790306	-0.0465471241
H	1.3711019898	2.4411932235	0.9038454038
H	0.7940033929	2.4573971672	-0.8188021043
C	-0.6181409138	0.7579556846	0.1433154342
H	-0.2825698665	0.4647023575	1.1363417519
C	-1.5996233184	1.9125462241	0.1086192953
C	-0.6056478913	-0.229276017	-0.8452526393
H	-1.3361372012	-0.1430749625	-1.6463183257
C	-0.115578369	-1.6250698116	-0.5186129304
H	2.7504436428	-0.5909095549	-1.7891972773
H	0.8248660263	-1.5348753552	0.0383681092
H	0.1256238212	-2.1673859436	-1.4409908377
C	-1.113825728	-2.4589018473	0.307618346
H	-0.6209967553	-3.3812839723	0.6454301002
C	-2.3886583047	-2.8306563069	-0.4598339277
H	-1.3793591436	-1.9029959024	1.2169056998
H	-2.1162285153	-3.4548542413	-1.3218758274
H	-2.8463766038	-1.9250127152	-0.8748811107
C	-3.4150692986	-3.5622781715	0.4086408222
H	-3.7388041826	-2.9309600383	1.2442806503
H	-2.9930489353	-4.4804012635	0.8334370245
H	-4.3060209478	-3.8380737458	-0.1650293514
C	-2.8140259946	1.7210693159	1.0441581404
H	-1.9402884228	2.0679143864	-0.923200845
H	-1.1108164472	2.8482763559	0.407228259
H	-2.4437602108	1.6452685436	2.0755993022
C	-3.7062013399	0.5071091093	0.7498857951
H	-3.4251646417	2.6336272293	1.0054691526
C	-4.3767682452	0.5392540048	-0.6266330912
H	-4.4814160184	0.4504461766	1.524735081
H	-3.1128540599	-0.4079168137	0.8445360792
H	-5.0432936071	-0.3189847684	-0.7608245158
H	-3.6401549967	0.510835182	-1.4357437872

H	-4.9729908318	1.450298717	-0.7551334523
C	3.4141908576	0.638003426	0.6143414191
C	4.3354781986	-0.4882095618	0.1109749865
H	5.1320345466	-0.668170407	0.8403024219
H	3.7923892583	-1.4294382994	-0.0227773723
H	4.8097379351	-0.2275341166	-0.8407864259
C	4.2828117723	1.8934340031	0.8605528854
H	4.7448525687	2.2341562401	-0.0718772021
H	3.687026218	2.7202171343	1.2583059239
H	5.08208364	1.6771148473	1.5789783055
C	2.7899057062	0.1825008291	1.9534691265
H	2.1800795688	-0.7162485179	1.8153379316
H	3.5754649519	-0.0498818287	2.6815719056
H	2.1522974233	0.9556367732	2.3917671258
H	2.1522974233	0.9556367732	2.3917671258

TS exo 0116

E(RB3LYP) = -706.415091843 A.U.

First frequency = -498.1060 cm^{-1}

H	0.6085584534	0.5145201852	-3.2920210988
C	0.803560172	0.9304043864	-2.3069999514
H	0.304481499	1.8732862387	-2.1164492941
C	1.9687048066	0.5775543982	-1.6438271418
C	2.2220440088	0.9534504663	-0.3066384342
C	1.2955024179	1.7816582995	0.3145133219
H	1.3862977422	2.0217971384	1.3695409549
H	0.7609288049	2.5275429583	-0.2594744948
C	-0.6761876487	0.6532875806	0.2429573728
H	-0.3177687748	0.0949161401	1.1032982182
C	-1.6049401299	1.8069317067	0.5568265754
C	-0.7388044938	-0.0245370987	-0.9769759055
H	-1.4899000309	0.3081566769	-1.6914098422
C	-0.3220713523	-1.4752741882	-1.0951785554
H	2.578331408	-0.1979394985	-2.0946009792
H	0.5981470236	-1.6277071766	-0.5163948097
H	-0.065552473	-1.6982965532	-2.1367864956
C	-1.3879692345	-2.4920673225	-0.6321120792

H	-2.3336184094	-2.2862663968	-1.1539081326
C	-1.641067941	-2.537345954	0.8789432525
H	-1.0752637632	-3.4926977773	-0.9624126758
H	-1.9710711202	-1.5542849702	1.2300383943
H	-0.692525118	-2.742550877	1.3947072609
C	-2.6826302979	-3.5896451918	1.2698879462
H	-2.3727633092	-4.592639632	0.9544872855
H	-3.6479667233	-3.3787431049	0.7952018714
H	-2.8429894089	-3.6145154638	2.352736949
C	-2.9701760552	1.3710801916	1.1373816215
H	-1.7623745108	2.4060968596	-0.349767613
H	-1.1352920514	2.4795553833	1.2844276684
H	-2.7858981393	0.7608504285	2.0318032711
C	-3.8912019015	0.5961747932	0.182724445
H	-3.4995233113	2.2694321892	1.4848685995
C	-4.3530008601	1.4060322044	-1.0334633886
H	-4.7720672826	0.2641193289	0.7467815842
H	-3.3861240444	-0.3144688544	-0.1568598799
H	-5.0578151451	0.8334089795	-1.6450669263
H	-3.5140124374	1.686600393	-1.6786522822
H	-4.853179965	2.3314895433	-0.7247271316
C	3.3429810273	0.3025290887	0.530558713
C	2.7265945726	-0.4954043304	1.7029483768
H	3.5158782876	-0.950094236	2.3125320849
H	2.1269801263	0.1408421774	2.3602954399
H	2.0799754716	-1.297765836	1.3328504503
C	4.2152022943	-0.6611912491	-0.2947429574
H	3.6383932671	-1.5127314794	-0.6699950785
H	4.6773615696	-0.1565557063	-1.1494599628
H	5.0206040621	-1.0591907121	0.3311403465
C	4.2597849739	1.4112268611	1.0971867264
H	3.7016828234	2.1088825446	1.7284031554
H	5.0637026136	0.9773571936	1.7031932741
H	4.7167635529	1.9880736071	0.2863731943
H	4.7167635529	1.9880736071	0.2863731943

TS_{exo} 0117

E(RB3LYP) = -706.414487654 A.U.

First frequency = $-515.4923 \text{ cm}^{-1}$

H	1.1478727194	0.1298992972	-3.3558838602
C	1.1008124668	0.6052907234	-2.379492822
H	0.5093110915	1.5139532089	-2.3594979763
C	2.1409346004	0.4083490996	-1.4828599489
C	2.0901193216	0.8673810389	-0.1480707208
C	0.9821618933	1.6135455601	0.2308837567
H	0.8294759519	1.915350258	1.2602059612
H	0.5038940768	2.2643652172	-0.4899334621
C	-0.821349201	0.293534402	-0.183950314
H	-0.6122558197	-0.211589763	0.7545847042
C	-1.8864283889	1.3676470933	-0.1319282936
C	-0.5826319724	-0.4138084681	-1.366996777
H	-1.2140497849	-0.1585429934	-2.2189900804
C	-0.0746693507	-1.8404890305	-1.3474694921
H	2.9003783825	-0.3227308094	-1.7490686242
H	0.6875753156	-1.9366620003	-0.5673836482
H	0.4343925537	-2.0642113688	-2.2918252736
C	-1.1776762459	-2.9032409805	-1.1443113937
H	-1.9335146882	-2.7763509848	-1.9313921914
C	-1.8787424064	-2.9046931563	0.2226214019
H	-0.7300407995	-3.8936353513	-1.3092541691
H	-2.6741603759	-3.6607601086	0.2006438274
H	-2.3780420896	-1.9427234728	0.3799638915
C	-0.9467277602	-3.1978589661	1.4031957314
H	-1.5061622119	-3.2669616085	2.3419175227
H	-0.1913363745	-2.4156275363	1.5298818475
H	-0.4142318118	-4.1455062598	1.2603669676
C	-3.3095205706	0.7963779178	0.0168117314
H	-1.8436237423	1.9661286669	-1.0541900964
H	-1.6844628317	2.0598061939	0.6929744376
H	-3.4842131895	0.0817417533	-0.7971400495
C	-4.4192643794	1.8593289251	0.0086435116
H	-3.3682191757	0.2180627132	0.9497348843
C	-4.379474684	2.8187212874	1.2038009347
H	-5.3917091878	1.3509184511	-0.0091554033
H	-4.3593876011	2.4346451477	-0.9256369128

H	-5.2280934579	3.5102393747	1.184613759
H	-3.465957106	3.4217208828	1.2123231403
H	-4.4202605425	2.2665742209	2.1500945849
C	3.1281076665	0.3433001875	0.865062946
C	3.0319031793	-1.1944645468	0.996749235
H	3.7874063181	-1.5694474067	1.696931316
H	2.0477669733	-1.4903095627	1.3746740582
H	3.1871613072	-1.6959525893	0.037495114
C	4.5419493465	0.7247044149	0.3692898376
H	5.303120687	0.3664762071	1.0719247412
H	4.7615452597	0.2889239751	-0.6095677821
H	4.6421510388	1.8112906639	0.2808349871
C	2.9336274987	0.9519853003	2.2659903042
H	3.7189488464	0.5938177406	2.9398087481
H	2.9853377313	2.0451454275	2.2404140006
H	1.9715755363	0.6652771333	2.7033441905
H	1.9715755363	0.6652771333	2.7033441905

TS exo 0119

E(RB3LYP) = -706.414419895 A.U.

First frequency = -512.4794 cm⁻¹

H	0.3278168073	-0.5723177458	-3.0316524736
C	0.6212255257	0.1539291331	-2.2779654439
H	0.251307482	1.1561039421	-2.4629413225
C	1.7867714714	-0.0574299914	-1.5559346278
C	2.1611466215	0.7529909608	-0.461073177
C	1.3544049176	1.8445435887	-0.168113599
H	1.524812159	2.4533846802	0.7117301121
H	0.8534396364	2.3695382975	-0.9713639991
C	-0.7271940647	1.0114722119	0.2025517244
H	-0.4025865143	0.7353527711	1.2041747125
C	-1.4993628069	2.3103210312	0.1098824077
C	-0.9295254698	-0.0324900338	-0.7066585024
H	-1.6820987874	0.1223866176	-1.4778305406
C	-0.7062119878	-1.4666316058	-0.2764617521
H	2.2915802744	-1.011498425	-1.6873173711
H	0.2574989351	-1.52982968	0.2429445508

H	-0.6221879272	-2.1103721639	-1.1583148215
C	-1.8064631703	-2.004700718	0.6567965815
H	-1.9180814483	-1.3142550839	1.5023071663
C	-1.5320167839	-3.4185941393	1.192703023
H	-2.7697981727	-1.9974216828	0.1271420177
H	-2.3003483283	-3.6696804132	1.9351677461
H	-0.5748261272	-3.4169230861	1.7324740647
C	-1.5066803925	-4.5063435999	0.1126548233
H	-0.6892504782	-4.3536063355	-0.5991082704
H	-2.4437591526	-4.5146043972	-0.4565174919
H	-1.376013443	-5.4998369539	0.5539568717
C	-2.8485820347	2.288906034	0.8635300862
H	-1.6672793435	2.55942183	-0.9462155784
H	-0.9046567445	3.1341986774	0.5225466753
H	-2.6525700301	2.033764576	1.9136983289
C	-3.9136854929	1.3320965657	0.3077535891
H	-3.2565871287	3.3095142666	0.8678291
C	-4.386111151	1.6777481683	-1.1084346442
H	-4.777186559	1.3457420644	0.9850101932
H	-3.527991014	0.3071578819	0.3254985818
H	-4.7670826896	2.704659088	-1.1578832078
H	-5.1894144285	1.0077031986	-1.431769112
H	-3.5762643577	1.5934195156	-1.8404346418
C	3.293813709	0.2789527651	0.47237647
C	3.5775683041	1.2866817736	1.6014558316
H	2.7173064932	1.4011393007	2.2691535403
H	4.4192640024	0.9379735427	2.2089091124
H	3.8358072479	2.2735335841	1.2043081797
C	2.9343508445	-1.0769051001	1.1237969203
H	3.7498179962	-1.4219614477	1.7700812202
H	2.0328906922	-0.9849414291	1.7387061307
H	2.7520741902	-1.8523176212	0.3744508519
C	4.5863455459	0.1162706798	-0.3602702812
H	5.4126258511	-0.2183560471	0.2774712008
H	4.4650083068	-0.61919044	-1.1607238735
H	4.8732428567	1.0668498228	-0.8213651367
H	4.8732428567	1.0668498228	-0.8213651367

TS exo 0120

E(RB3LYP) = -706.415593249 A.U.

First frequency = -500.6069 cm⁻¹

H	1.3181018928	-0.6448719987	-3.4229640223
C	1.3262405313	0.0528885016	-2.5897086003
H	0.8793472706	1.0149235819	-2.8117914081
C	2.2826477337	-0.0928294978	-1.5968913056
C	2.2687345873	0.6763983268	-0.4127741586
C	1.3029036007	1.6683878043	-0.3023156084
H	1.1768339395	2.2205628277	0.6241081051
H	0.9713828518	2.2061574495	-1.1811045807
C	-0.6962676322	0.5943797137	-0.5074648082
H	-0.5843107727	0.3337371686	0.5397973712
C	-1.5665418127	1.7970138578	-0.8104691247
C	-0.5472323462	-0.4309075443	-1.4433618713
H	-1.0964416665	-0.3283972056	-2.3797068685
C	-0.2464086933	-1.8528540793	-1.017784966
H	2.9082439523	-0.9777329044	-1.6396556532
H	0.413600777	-1.8287403944	-0.1430968545
H	0.3191542134	-2.3664585106	-1.803026123
C	-1.5002822779	-2.7031478931	-0.7146351192
H	-2.1194151758	-2.7415357952	-1.6213200061
C	-2.3733747005	-2.2365204158	0.4589196548
H	-1.1737451569	-3.7355377601	-0.5253208144
H	-3.2557054627	-2.887090399	0.5135753245
H	-2.7500493663	-1.2301590004	0.2515751705
C	-1.6632941944	-2.2470471814	1.8164145834
H	-2.3486356076	-1.9647099785	2.62248249
H	-0.8220063815	-1.5474880779	1.8428139319
H	-1.2679001893	-3.2432323833	2.0473737686
C	-3.0605291986	1.5681728736	-0.5024550266
H	-1.4556232874	2.0540009834	-1.8727171256
H	-1.2266463234	2.6741519736	-0.2446934502
H	-3.6464250537	2.3992795052	-0.9189139832
C	-3.3698427591	1.4503248067	0.9956090024
H	-3.398151943	0.6617865879	-1.0226770172
C	-4.83831791	1.1189186146	1.2732854799

H	-3.0995859826	2.3933056055	1.4902144799
H	-2.7347088977	0.6790808905	1.4476383929
H	-5.1093229405	0.1528418379	0.83200517
H	-5.5039385383	1.8763830389	0.8435985566
H	-5.0433274124	1.0640880565	2.3473898925
C	3.1183080105	0.2999972251	0.8192937989
C	3.9592041611	1.5243274013	1.2489695449
H	3.3245097102	2.3779366948	1.5039721675
H	4.5705322946	1.2852258796	2.1269093297
H	4.6291538856	1.8369186095	0.4412341827
C	2.1929481477	-0.1157407738	1.9862231841
H	1.6031346837	-0.999015648	1.7206042268
H	2.7844255244	-0.3602198825	2.8759769647
H	1.4968796849	0.6822976641	2.260487579
C	4.0843291338	-0.865720611	0.5388324894
H	4.6968146672	-1.0600256731	1.4253605098
H	3.5490230888	-1.7903093876	0.2999456663
H	4.7621028933	-0.6376172658	-0.2902664122
H	4.7621028933	-0.6376172658	-0.2902664122

TS exo 0122

E(RB3LYP) = -706.414002539 A.U.

First frequency = -521.6848 cm⁻¹

H	0.7854091636	-1.4614686685	-2.6556796309
C	0.9792975144	-0.531194507	-2.1275249687
H	0.5613039346	0.3444773112	-2.6113733703
C	2.1117874419	-0.434653675	-1.3296985131
C	2.3604482305	0.6776451174	-0.4965746212
C	1.4603709021	1.7335685693	-0.5574390898
H	1.5287595612	2.5754462616	0.1212538053
H	0.9782752152	1.9690304461	-1.4974453079
C	-0.58665494	0.86397318	-0.0695870205
H	-0.3168646587	0.9176113737	0.9836355471
C	-1.4367254094	2.0117729164	-0.5757636371
C	-0.6406781311	-0.4114267961	-0.6464126183
H	-1.3500128716	-0.5514524481	-1.4603089204
C	-0.334147896	-1.6335385271	0.1975830811

H	2.6870630903	-1.342328622	-1.1640439273
H	0.5178534421	-1.3953036222	0.8429489915
H	-0.0044830383	-2.4633703421	-0.4365263198
C	-1.5104611515	-2.1001549439	1.0795424701
H	-1.1440040723	-2.8643070893	1.77955608
C	-2.7072679742	-2.680151114	0.3066531177
H	-1.8473209063	-1.2552455196	1.6938282729
H	-3.0815867417	-1.9379399368	-0.4087848779
H	-3.5279462105	-2.8576720711	1.0133783366
C	-2.3948708443	-3.9846465591	-0.4355056836
H	-2.0113148115	-4.746863241	0.2528056392
H	-1.6420118708	-3.8376432313	-1.2167596309
H	-3.2908201426	-4.3899457239	-0.9169707264
C	-2.7763147762	2.1818013515	0.1707471331
H	-1.6363705364	1.8691373879	-1.6474381768
H	-0.889430759	2.95853253	-0.4904402158
H	-2.572170345	2.3174005794	1.2425285846
C	-3.7661781717	1.0282502469	-0.0105563019
H	-3.246558362	3.1153192201	-0.1686449534
C	-5.1001639097	1.2708815306	0.7006116961
H	-3.3148551801	0.1050268814	0.3638307793
H	-3.9419470947	0.8683834238	-1.0837355198
H	-5.5949320089	2.1725519042	0.3214951122
H	-4.951661475	1.4059094633	1.7782680019
H	-5.7872145662	0.4295824402	0.5625238265
C	3.4662338805	0.5833711436	0.5745609025
C	3.6155721898	1.8916533068	1.3727377583
H	4.442883409	1.8013591744	2.0844125318
H	3.8280816201	2.7412394348	0.7159568133
H	2.7128127647	2.1217738191	1.9480707953
C	3.1615808844	-0.5543538509	1.5763613385
H	3.9636958014	-0.6389693257	2.3188063263
H	2.2266751521	-0.3591960622	2.1120613575
H	3.066321687	-1.5219375117	1.0757277363
C	4.8129685225	0.2952931594	-0.1281210826
H	5.6216147176	0.227389769	0.6086821781
H	4.7893372643	-0.6466216059	-0.6835918108
H	5.0605049702	1.0934776693	-0.8353220733

H 5.0605049702 1.0934776693 -0.8353220733

TS exo 0127

E(RB3LYP) = -706.413847094 A.U.

First frequency = -481.8023 cm^{-1}

H	0.5743626507	-0.4187043134	-3.186673671
C	0.7272808716	0.246501332	-2.3411187816
H	0.1992934373	1.1898445386	-2.4135987625
C	1.865041984	0.1053521422	-1.5661194887
C	2.0644118315	0.8249980284	-0.3651887763
C	1.111136069	1.7701585294	-0.0124299442
H	1.1636627436	2.2816990817	0.9437878257
H	0.5795475324	2.3222678443	-0.7766355434
C	-0.8505862694	0.6142357284	0.1630481455
H	-0.5179925541	0.30359542	1.1510099337
C	-1.8128156504	1.7799413894	0.1311028644
C	-0.8688241627	-0.3551058506	-0.8366358499
H	-1.5984296094	-0.2350333918	-1.6364133876
C	-0.4279236685	-1.7688950627	-0.5355565049
H	2.501855584	-0.7471390907	-1.7758217879
H	0.5296400851	-1.7317046318	0.0014102185
H	-0.234945328	-2.3076649158	-1.4690813063
C	-1.4482140327	-2.5452276431	0.3180834876
H	-1.6625552279	-1.961568205	1.2220843002
C	-0.9837932254	-3.9530084137	0.7222749317
H	-2.3989374111	-2.6164615151	-0.2292649733
H	-1.7141385665	-4.3777415083	1.4228995412
H	-0.0392742032	-3.8724226567	1.2783843825
C	-0.8017232663	-4.917893938	-0.4550871822
H	-0.5358252636	-5.9215993274	-0.107548276
H	-0.0103180114	-4.5857735619	-1.1344418105
H	-1.7257473082	-5.0009809367	-1.039367094
C	-3.2058812206	1.3971681872	0.6669136772
H	-1.9014369301	2.1436308606	-0.9010897204
H	-1.4257674751	2.6199385202	0.7226690135
H	-3.6192819742	0.5963201158	0.0391137128
C	-4.1993282212	2.5669567785	0.7351808655

H	-3.0870907716	0.9656343939	1.6697112466
C	-4.5656584371	3.1556485919	-0.632129774
H	-3.7830146525	3.3574688743	1.3748094575
H	-5.1145384803	2.2229101965	1.2336992454
H	-3.6977506531	3.6004642923	-1.1294057348
H	-5.325022758	3.938501739	-0.5361246564
H	-4.9666267126	2.3812844086	-1.2966902381
C	3.1624808861	0.4372914767	0.6479933818
C	4.0752965291	-0.6898529626	0.1310464149
H	3.5225848848	-1.6216388993	-0.026933554
H	4.5625024943	-0.4159647939	-0.810427521
H	4.8618773918	-0.8942571359	0.8647508432
C	4.0456477945	1.6735548885	0.9351125428
H	4.8323548539	1.4282791748	1.6580747847
H	4.5245529138	2.0293536529	0.0169354372
H	3.4575716926	2.4996802469	1.3453067982
C	2.513533216	-0.0412393282	1.9673462022
H	1.8916880418	-0.926513398	1.7984164334
H	3.2853099402	-0.3039046165	2.6999574602
H	1.8816726603	0.7308952685	2.4156715895
H	1.8816726603	0.7308952685	2.4156715895

TS exo 0137

E(RB3LYP) = -706.415245624 A.U.

First frequency = -504.5659 cm⁻¹

H	1.281901128	-1.5145357553	-2.7401397278
C	1.2444148089	-0.5696239524	-2.2043840983
H	0.7242382301	0.2201454488	-2.7346463739
C	2.2310532068	-0.2806352143	-1.2749191286
C	2.1763870358	0.8514284608	-0.4296691164
C	1.1256134223	1.7394277211	-0.6125690445
H	0.9692745746	2.575895161	0.0579332851
H	0.7217184237	1.8937107901	-1.6047772038
C	-0.7727942294	0.514197202	-0.3379954038
H	-0.6244858203	0.5957633065	0.7357445179
C	-1.7414350838	1.5019097822	-0.9532498773
C	-0.5661916074	-0.7404123076	-0.915610816

H	-1.1420509955	-0.9660969649	-1.8121938101
C	-0.1735998641	-1.9243650178	-0.0570946001
H	2.9360436666	-1.0715917503	-1.030782763
H	0.6851068471	-1.6386585151	0.560014013
H	0.1704631644	-2.7481558779	-0.6922655642
C	-1.2986506599	-2.4218215756	0.8746274254
H	-0.9217011288	-3.2794115855	1.4497541774
C	-2.5995866288	-2.8257844401	0.1643660839
H	-1.5236262309	-1.6345435923	1.6055993343
H	-3.0309212592	-1.9448422993	-0.3264654285
H	-3.3298644053	-3.1394835633	0.9210519896
C	-2.4245268292	-3.9468501566	-0.8655569319
H	-1.7818944854	-3.634818372	-1.6956107392
H	-3.3871131433	-4.2487525155	-1.2910346798
H	-1.9672312343	-4.8333831664	-0.410599063
C	-3.2250608969	1.1647890254	-0.6893730162
H	-1.5847158323	1.5309564918	-2.0404325948
H	-1.5305333436	2.514287074	-0.5902670154
H	-3.847373816	1.9454855916	-1.1490812409
C	-3.6021211588	1.0282490705	0.7936616236
H	-3.4695928106	0.2278405498	-1.2055460805
C	-3.3140011611	2.2809236627	1.6279367009
H	-3.0681078906	0.1727564321	1.2244104275
H	-4.6698311199	0.7845572804	0.8612900641
H	-2.2412194622	2.4966982466	1.6742851401
H	-3.6693117666	2.1622597245	2.6566388858
H	-3.8090819567	3.1618931416	1.2027222327
C	3.1370138351	0.9357719463	0.7739446399
C	4.5916597825	0.9055419878	0.2511473462
H	4.8062559469	-0.0128862354	-0.3027370946
H	4.7812733827	1.7508385813	-0.4182212391
H	5.2993439547	0.964337251	1.0860865089
C	2.9471189806	2.2334489017	1.580839259
H	3.6795015587	2.2766215254	2.3936997155
H	3.0871932714	3.1206192836	0.9550547208
H	1.9517652835	2.2881490903	2.034006864
C	2.9153962052	-0.2573759288	1.7326499371
H	1.8949057167	-0.251460193	2.1297998431

H	3.0754613947	-1.2162242289	1.2316656303
H	3.6081564579	-0.2041648307	2.5805667999
H	3.6081564579	-0.2041648307	2.5805667999

TS exo 0140

E(RB3LYP) = -706.414918870 A.U.

First frequency = -492.4464 cm⁻¹

H	0.1965007913	-1.2635731534	-2.7381979069
C	0.4818243201	-0.418203566	-2.1192621365
H	0.0522924004	0.5255460589	-2.4321814487
C	1.6465377756	-0.4831288803	-1.3755246627
C	2.0177969668	0.5201649214	-0.4514971476
C	1.2211399568	1.6583686834	-0.3850950375
H	1.4112466679	2.4227815071	0.3623546529
H	0.7450072079	2.0352719771	-1.2813128036
C	-0.8491380106	0.9587512951	0.1616811782
H	-0.5325249673	1.0016852113	1.20157364
C	-1.6554412204	2.141846886	-0.3260717851
C	-1.0415425461	-0.3074595686	-0.3865322701
H	-1.802233278	-0.4241900199	-1.1565158319
C	-0.6832502052	-1.531759969	0.4216082467
H	2.162310929	-1.4371269712	-1.3495955649
H	-1.2646100369	-1.523133796	1.3566586639
H	0.3686416031	-1.4453412996	0.7300775134
C	-0.9007457929	-2.8725973571	-0.2819209746
H	-1.9490984284	-2.9508105819	-0.6041485557
C	-0.5479483998	-4.075719583	0.5990460652
H	-0.2969809849	-2.9071681847	-1.1965673806
H	-1.1508465158	-4.0449240222	1.5168726133
H	0.4990501856	-3.9884800209	0.9212690635
C	-0.7568401398	-5.4173318665	-0.1086147896
H	-0.4955304013	-6.2605532889	0.5390402905
H	-0.1395951222	-5.4860114768	-1.0117783503
H	-1.8019435381	-5.5424503491	-0.4143971447
C	-3.0747640886	2.1801151751	0.2674800334
H	-1.7284240843	2.1069456185	-1.4228318512
H	-1.1439436548	3.0819299858	-0.0825049574

H	-3.5981655368	1.2512943465	0.0041212111
C	-3.8951459332	3.3863448203	-0.2026715656
H	-3.006984533	2.1888193742	1.3644587357
C	-5.3070964151	3.4156523701	0.3895147798
H	-3.9554865189	3.3761469514	-1.2996614932
H	-3.3644088013	4.3107821416	0.0631332098
H	-5.8735287052	4.2846152019	0.038965702
H	-5.2739493583	3.4579662804	1.4842175329
H	-5.8689843614	2.5164850506	0.1120182294
C	3.1360920853	0.3065271864	0.5899647562
C	4.2237955166	1.3862748152	0.3824651338
H	5.0340747323	1.2671492022	1.1113129094
H	4.6544033593	1.3150238014	-0.6217840829
H	3.811204002	2.3930691598	0.4971741401
C	2.5639050338	0.4340111629	2.020600811
H	1.8004699054	-0.3279106811	2.2069440549
H	3.3607083318	0.3041759274	2.761792647
H	2.1094519305	1.4132936977	2.1955798852
C	3.8034321676	-1.0757522818	0.4687586818
H	4.2503427136	-1.2253238001	-0.5193833324
H	4.6037635457	-1.1666980147	1.2103855781
H	3.09099819	-1.8876760377	0.6494435397
H	3.09099819	-1.8876760377	0.6494435397

TS exo 0143

E(RB3LYP) = -706.414307695 A.U.

First frequency = -482.4956 cm⁻¹

H	0.7441038207	-0.7932064441	-3.0300578441
C	0.8489358118	-0.0343111739	-2.2593604966
H	0.2100251215	0.8303485691	-2.3940423135
C	2.02470405	0.0341878149	-1.5324942729
C	2.1819252319	0.8857371538	-0.414692758
C	1.1353647133	1.7433430019	-0.1038759232
H	1.1632322617	2.3492621531	0.7965957358
H	0.5151504742	2.154287057	-0.8898602158
C	-0.6676916446	0.3990129539	0.2729750839
H	-0.2699508504	0.227888772	1.2708311943

C	-1.7552255525	1.4448502854	0.1707406271
C	-0.6060394995	-0.6617042997	-0.6280429591
H	-1.3696751578	-0.7027776658	-1.4027517074
C	0.0175850298	-1.9761357033	-0.2153099204
H	2.7512280265	-0.754703733	-1.6937433161
H	0.9925874484	-1.7682121863	0.2426767653
H	0.2244533362	-2.5893247059	-1.0990898769
C	-0.8359802267	-2.7784800177	0.7891212349
H	-0.2931988265	-3.6963970754	1.0559636978
C	-2.2400268408	-3.1527100741	0.2892849909
H	-0.9337379284	-2.1936430349	1.7126879772
H	-2.8142292809	-2.2355210697	0.1083862824
H	-2.7661234555	-3.6874225804	1.0902955468
C	-2.2430423312	-4.0135606162	-0.9785543223
H	-1.8209251675	-3.4752893886	-1.833739137
H	-3.2597808305	-4.3154144949	-1.2504816889
H	-1.6501368321	-4.9250705769	-0.8381453284
C	-3.0836646773	0.9732610071	0.7927676346
H	-1.9124533224	1.6963279751	-0.8864298897
H	-1.445700037	2.3742949447	0.6664511564
H	-3.4385847989	0.0897654685	0.2455042736
C	-4.1858930887	2.0431223099	0.8112863315
H	-2.8890715117	0.6366064966	1.8196474482
C	-4.6517384765	2.4828622113	-0.5814952437
H	-3.8300127473	2.9184406447	1.3720826519
H	-5.0459952458	1.652790071	1.3701284181
H	-4.9936405949	1.6227671207	-1.1692513028
H	-3.8485711274	2.969169314	-1.1443734153
H	-5.482332404	3.1931158757	-0.5158370655
C	3.3582034196	0.7317438006	0.5727047927
C	4.3785795261	-0.3284557727	0.1191716011
H	4.7921130865	-0.0956015523	-0.8675019329
H	5.2121955801	-0.3660973002	0.8280197388
H	3.9359499521	-1.3289919701	0.078273124
C	4.0969737541	2.084735061	0.6940210596
H	4.4923936601	2.3989609917	-0.277526258
H	3.4306104292	2.8743653736	1.0532597673
H	4.9358478783	2.0065587539	1.3953719729

C	2.8248909345	0.3175451352	1.9636222988
H	2.3075191035	-0.6460644731	1.9127624116
H	3.6514568222	0.2214623661	2.676979969
H	2.1234528435	1.0529737801	2.3680323518
H	2.1234528435	1.0529737801	2.3680323518

TS exo 0144

E(RB3LYP) = -706.414505056 A.U.

First frequency = -513.0339 cm⁻¹

H	0.1966582971	-1.3042199124	-2.6067995158
C	0.5406668941	-0.4249810508	-2.0704711163
H	0.2388149498	0.5116627972	-2.524110977
C	1.6801307609	-0.5106088283	-1.2866022435
C	2.1240043373	0.5515165253	-0.4669178562
C	1.4197767405	1.7477651076	-0.5356814055
H	1.6445178522	2.5739113214	0.1285090277
H	0.9847319971	2.0539444972	-1.4784995678
C	-0.7279925039	1.2743724057	-0.0168748049
H	-0.4497028671	1.3462764917	1.032920328
C	-1.3967612522	2.5052118	-0.5905898564
C	-1.0188836495	-0.0027385097	-0.5041803368
H	-1.7577364143	-0.0802298071	-1.2997034371
C	-0.8957206758	-1.1930623733	0.4215501032
H	2.1086609873	-1.4980808658	-1.1309854732
H	-1.5924418213	-1.0519443099	1.2629173338
H	0.1067754804	-1.1861088161	0.866728267
C	-1.168232362	-2.5607855989	-0.2080931685
H	-2.1521076923	-2.5491983481	-0.69912571
C	-1.1215695605	-3.7055956732	0.8098249132
H	-0.4343690623	-2.7554552398	-0.998869718
H	-1.8607905981	-3.5200715887	1.6009939152
H	-0.1409027279	-3.7045056756	1.3054625148
C	-1.3768066288	-5.0774330997	0.17949116
H	-1.3371082872	-5.8781652333	0.9251675691
H	-0.6303416205	-5.3015340978	-0.5912405736
H	-2.3629507763	-5.1140282232	-0.2976012264
C	-2.7415054303	2.8484757299	0.0852526267

H	-1.5623172138	2.3594778325	-1.6677997326
H	-0.7384717398	3.3775877982	-0.4958798271
H	-2.5718444851	2.9986201658	1.1609932314
C	-3.8473635141	1.8055072752	-0.1085606064
H	-3.0900777321	3.8150265813	-0.3046901848
C	-5.1740923586	2.2259331399	0.5304969937
H	-3.5233046065	0.8467247913	0.3123391848
H	-3.9936620364	1.631023869	-1.1837699993
H	-5.9497076379	1.4671837418	0.383522962
H	-5.5408390642	3.1657497104	0.1018450218
H	-5.059096747	2.3799445422	1.6096886766
C	3.2287737302	0.2877636883	0.5767775255
C	3.5752591701	1.5492204883	1.3886122605
H	3.9007015118	2.3688834359	0.7401797734
H	2.721599292	1.8982979824	1.9790171595
H	4.3898300751	1.3304252702	2.0869288489
C	2.8029812867	-0.8154645032	1.5730539245
H	1.9227485418	-0.5038730483	2.1446500663
H	2.5595946744	-1.7525401295	1.0642195621
H	3.6105046777	-1.0229642119	2.2847887445
C	4.504809635	-0.1688649603	-0.1685020401
H	5.3168860628	-0.3584785279	0.5429437771
H	4.3359711107	-1.0892411827	-0.7350642592
H	4.8389726924	0.5997644332	-0.872762867
H	4.8389726924	0.5997644332	-0.872762867

TS exo 0147

E(RB3LYP) = -706.414458883 A.U.

First frequency = -490.1520 cm^{-1}

H	0.3563597874	-0.3273506139	-3.1474611452
C	0.6398400322	0.333329159	-2.3324410805
H	0.2495252658	1.3403310376	-2.419094814
C	1.7861268776	0.0559647416	-1.6056827617
C	2.1383671983	0.7710933978	-0.4391028892
C	1.3394114614	1.8491731806	-0.079988639
H	1.5047879972	2.3752868022	0.8553257159
H	0.8647414659	2.4521058069	-0.8433149581

C	-0.7522992321	1.0046137305	0.2121384603
H	-0.4285680008	0.6880550113	1.2017338427
C	-1.5357329324	2.2987691699	0.171792961
C	-0.9360217544	0.0038909905	-0.7427141521
H	-1.6776428342	0.1784260361	-1.5192580653
C	-0.651673813	-1.4393558132	-0.392795893
H	2.2873475523	-0.8829658957	-1.8142535183
H	0.3330202313	-1.4929617529	0.0908149617
H	-0.575434291	-2.0357673338	-1.3078370986
C	-1.6995281826	-2.0598578248	0.5500258579
H	-1.8074187157	-1.412683332	1.4294086735
C	-1.3564934602	-3.4849550311	1.0110863941
H	-2.6796209423	-2.0640645	0.0521595169
H	-2.0905971492	-3.7983400021	1.7643834161
H	-0.3830961458	-3.4710697922	1.5211539385
C	-1.325906673	-4.5210390809	-0.1184420279
H	-2.2799293685	-4.5393526786	-0.658455088
H	-1.1446139725	-5.5277345112	0.2720982417
H	-0.5381031728	-4.3051384599	-0.8470784774
C	-2.8778747804	2.2324186487	0.9353672133
H	-1.7145240731	2.5842145329	-0.8731636528
H	-0.9463450514	3.1130567162	0.6104439081
H	-2.6677492891	1.9540817623	1.9768949319
C	-3.9273407776	1.2677182494	0.3635345217
H	-3.3060736562	3.2440909039	0.9694004641
C	-4.4206056964	1.6413784114	-1.0383360358
H	-4.7843873519	1.2438110719	1.048641177
H	-3.5185260866	0.2513113999	0.3496524423
H	-3.6155629538	1.5969995705	-1.7790343916
H	-4.8260893435	2.6599127383	-1.0554648182
H	-5.2107954935	0.9617482632	-1.3737417995
C	3.2193662314	0.264667721	0.5389771563
C	2.5788476367	-0.0648963463	1.9072118655
H	3.3433194942	-0.4067592226	2.6143121427
H	2.0866060024	0.8061565033	2.3491739289
H	1.8305969572	-0.8580919082	1.8081854643
C	3.9324933998	-1.0017886295	0.0308316652
H	4.7159875193	-1.2937750885	0.7377142323

H	3.2428832177	-1.8469134877	-0.0641364862
H	4.4078685191	-0.835830351	-0.9413797566
C	4.283925023	1.3697390783	0.7302265433
H	5.0639488837	1.040506027	1.426599018
H	4.7605330298	1.6180927271	-0.223790413
H	3.8411391525	2.2868162115	1.1297343841
H	3.8411391525	2.2868162115	1.1297343841

TS exo 0148

E(RB3LYP) = -706.415004751 A.U.

First frequency = -520.7219 cm^{-1}

H	0.4997222935	0.2761857282	-3.2509835995
C	0.7133798288	0.7209536851	-2.2823016084
H	0.2847246003	1.7080423513	-2.1477128222
C	1.8692875878	0.3463988523	-1.6102577755
C	2.147116574	0.7626714842	-0.2904925635
C	1.2549177364	1.6481099873	0.3014075494
H	1.3499319502	1.9341370197	1.3421549643
H	0.7544271725	2.3881894899	-0.3098163831
C	-0.7775000376	0.6376564304	0.2391287867
H	-0.4778206654	0.0779098536	1.1207866772
C	-1.6262251938	1.8634409868	0.5038931144
C	-0.8663811967	-0.0669538759	-0.9686504939
H	-1.5972197359	0.2935802144	-1.6912114832
C	-0.5706431524	-1.5515195671	-1.0334496934
H	2.4459399069	-0.4768742065	-2.0247828945
H	0.3250540241	-1.7610255005	-0.4395585825
H	-0.3178543964	-1.8292214541	-2.0629931775
C	-1.7323754737	-2.460681803	-0.572659818
H	-2.6259840406	-2.2126966133	-1.1615486785
C	-2.0885918024	-2.4136936679	0.9215054636
H	-1.4757613399	-3.4969810614	-0.8346117326
H	-2.9641825366	-3.0548737916	1.0855740267
H	-2.3993366537	-1.4005764317	1.1977114172
C	-0.9567364205	-2.8687253985	1.8488663825
H	-0.0969914239	-2.1927443745	1.8025209022
H	-0.6007367482	-3.8694502433	1.5774648664

H	-1.2891023923	-2.9032192915	2.891541608
C	-3.0473696315	1.5537375925	1.028086572
H	-1.6957568987	2.4627546913	-0.4137462556
H	-1.1330931537	2.5044722096	1.2443083885
H	-2.9567106583	0.9292071604	1.9269352373
C	-3.9997485351	0.8707695891	0.0346134303
H	-3.5041891259	2.4974221371	1.3580647044
C	-4.3306860525	1.7200674375	-1.1973858138
H	-4.9311149444	0.6280231268	0.5618508135
H	-3.5744795478	-0.0860674887	-0.2862503278
H	-4.7470292897	2.6918061837	-0.9069419596
H	-5.065343851	1.2194382884	-1.8364042203
H	-3.4437712529	1.9136456492	-1.8097234056
C	3.281749107	0.0709519421	0.4924797785
C	3.4400273228	0.6408711627	1.9139739979
H	2.5480596374	0.4630958756	2.523836219
H	4.2830631445	0.1563451118	2.417518089
H	3.6333401306	1.7181770229	1.8966994513
C	3.0177095514	-1.447484965	0.6158722572
H	3.8424134693	-1.9401187282	1.1438612616
H	2.0984164679	-1.6366901248	1.1792826685
H	2.9154507138	-1.9248857579	-0.3625390906
C	4.6105126245	0.2957171254	-0.2656199713
H	5.4408732968	-0.1815871983	0.2674572775
H	4.5778436157	-0.1234790916	-1.2753999782
H	4.830334175	1.3644510452	-0.3551127139
H	4.830334175	1.3644510452	-0.3551127139

TS exo 0150

E(RB3LYP) = -706.414838293 A.U.

First frequency = -512.5057 cm^{-1}

H	0.3036056194	-1.018640489	-2.8601925509
C	0.5357557255	-0.2375730782	-2.1425558299
H	0.1364098203	0.7347201792	-2.4062610745
C	1.6592957539	-0.3622412101	-1.3424508407
C	1.9642341911	0.5496523614	-0.306210171
C	1.1347083643	1.6557424134	-0.1633853059

H	1.2549228906	2.3474779434	0.6619261932
H	0.690406893	2.102919033	-1.0434966395
C	-0.9561366098	0.8662919756	0.1533328093
H	-0.7150594167	0.7601561853	1.2088787439
C	-1.7396404884	2.1063157085	-0.2157119551
C	-1.1007719886	-0.3108559541	-0.5831206033
H	-1.8103779157	-0.3038338818	-1.4097451892
C	-0.8534881592	-1.6421452225	0.0899945063
H	2.1930217129	-1.3094470605	-1.3713997281
H	-1.5651634409	-1.7515229009	0.9237705933
H	0.1393193459	-1.6079151233	0.5517352795
C	-0.9751937005	-2.8726545498	-0.8139942839
H	-1.9499494874	-2.8472199773	-1.3202057553
C	-0.8285264078	-4.2075246765	-0.0681838293
H	-0.2171497693	-2.8221883925	-1.604598584
H	-1.0429040349	-5.0275908196	-0.765225627
H	-1.5911711798	-4.2703842205	0.7202542253
C	0.5599005797	-4.4238517542	0.5460475774
H	0.782045723	-3.6838225194	1.3209380228
H	1.341794893	-4.3436030657	-0.2187970044
H	0.6422247191	-5.4151213347	1.0036263752
C	-3.1971570775	2.0579752757	0.2760198021
H	-1.7367521957	2.2283149142	-1.3088039978
H	-1.2570471	3.0029675999	0.1940538458
H	-3.6913830018	1.1766117663	-0.1541410312
C	-3.9956288147	3.3190483725	-0.0722830618
H	-3.2058427521	1.9086142585	1.3648981912
C	-5.4456393847	3.2618766687	0.4169557695
H	-3.9792644839	3.46727658	-1.1608106096
H	-3.4945687707	4.1956826104	0.3605661782
H	-5.977281411	2.4120364966	-0.0261747925
H	-5.9954680338	4.1721587042	0.1563515567
H	-5.4892687349	3.1454768517	1.505908795
C	3.0708858037	0.1951321781	0.7082784501
C	4.4055193023	0.0471731807	-0.0593889292
H	4.3548690248	-0.7464481536	-0.8105344568
H	4.6621450589	0.9783568388	-0.5746593185
H	5.2201456012	-0.1980666835	0.6318696912

C	3.2528487115	1.2881317497	1.777174121
H	3.4967258691	2.2556754248	1.3270596148
H	2.3520870498	1.411974922	2.3874972103
H	4.0716206118	1.0163489721	2.4515442523
C	2.7576014333	-1.1329232088	1.435810509
H	3.5695681073	-1.3947386622	2.1241507887
H	1.8358908815	-1.0471846817	2.0207803144
H	2.6348724675	-1.9635716016	0.7356744626
H	2.6348724675	-1.9635716016	0.7356744626

TS exo 0151

E(RB3LYP) = -706.414378465 A.U.

First frequency = -495.2024 cm⁻¹

H	1.1026364789	0.0382233569	-3.4141369321
C	1.0844993958	0.5316491755	-2.4459678301
H	0.4890467271	1.4369250715	-2.4194729498
C	2.1330642851	0.3262597192	-1.5636931088
C	2.1149298959	0.8105782055	-0.2368000663
C	1.0316209303	1.5883847834	0.1507169767
H	0.9135100534	1.8999942169	1.1841823062
H	0.5482540734	2.2431787978	-0.5624989992
C	-0.8187689619	0.2913880044	-0.1965851781
H	-0.5995166436	-0.1712256907	0.7612420698
C	-1.8607720948	1.388230341	-0.178208598
C	-0.6053338538	-0.4697678213	-1.3458176193
H	-1.2348795025	-0.2475682023	-2.2077623222
C	-0.0829234995	-1.887745449	-1.2688818703
H	2.8723162459	-0.4179377303	-1.8392698474
H	0.6786350768	-1.9433223118	-0.4824904959
H	0.4313885046	-2.1454270525	-2.2014262058
C	-1.1781972763	-2.9503700283	-1.0248691207
H	-1.9228015671	-2.870799587	-1.8286449711
C	-1.9009342152	-2.8866046894	0.3291327012
H	-0.7196862547	-3.943674916	-1.1322261103
H	-2.6973386157	-3.6419311014	0.329545571
H	-2.4005338862	-1.9172513379	0.4322663503
C	-0.9891707902	-3.1247249929	1.537487267

H	-1.5647826142	-3.1492812202	2.4686605783
H	-0.2350357275	-2.3385351528	1.6410842548
H	-0.4572416222	-4.0793706291	1.4484715933
C	-3.2914345876	0.8503065925	0.0161003124
H	-1.820513084	1.9448385971	-1.126359751
H	-1.6331022353	2.111288721	0.6128035132
H	-3.4924796436	0.1080578226	-0.7664361777
C	-4.3819479483	1.9324574775	-0.0155521849
H	-3.3442839633	0.3093388784	0.9715485089
C	-4.3056093082	2.93571803	1.1411792766
H	-5.363479543	1.4417916452	0.0013327939
H	-4.327045206	2.4705825171	-0.9720338874
H	-4.3414146671	2.4208494276	2.1084540158
H	-5.1416349007	3.6419049369	1.1083845888
H	-3.3812134068	3.5212930453	1.1126743808
C	3.1241600254	0.3249663422	0.8252501053
C	2.3892804723	-0.4908672107	1.9131384753
H	1.5979021914	0.0904411799	2.3952541618
H	1.9329832583	-1.3882671816	1.4834945273
H	3.0901553448	-0.8095081783	2.69326786
C	4.2299269762	-0.5647732123	0.2279277835
H	4.7813756367	-0.0465745872	-0.5633927821
H	4.946731725	-0.8382572557	1.0091144794
H	3.8263045594	-1.4938940557	-0.1870876506
C	3.8014034836	1.551482508	1.4795707662
H	3.069717466	2.2038686539	1.9647631233
H	4.5249775714	1.2341929329	2.2394380656
H	4.3326525727	2.1466859317	0.7295869967
H	4.3326525727	2.1466859317	0.7295869967

TS exo 0152

E(RB3LYP) = -706.414874767 A.U.

First frequency = -494.0147 cm⁻¹

H	0.1999856137	-1.2002902075	-2.7400552033
C	0.5468777752	-0.3536032724	-2.1552640067
H	0.2309121923	0.6086421459	-2.5388121607
C	1.6719074218	-0.4923776298	-1.3609623718

C	2.1079921951	0.51910604	-0.4757744426
C	1.4254611222	1.7310060356	-0.5020669668
H	1.6619044263	2.5140868736	0.21213947
H	1.023511189	2.1013623361	-1.4365324572
C	-0.7208373302	1.272776104	-0.0045019102
H	-0.4363572057	1.3322773622	1.0443775091
C	-1.3908758362	2.5109890979	-0.5607559388
C	-1.0133048026	0.0033037261	-0.5029922333
H	-1.7536416317	-0.0792057598	-1.2955666571
C	-0.8112992114	-1.2047868716	0.3811741446
H	2.0857376063	-1.4903125425	-1.2621315767
H	-1.4209157331	-1.0856643953	1.2903917302
H	0.2322308212	-1.2087428271	0.7275211343
C	-1.1432610222	-2.553019103	-0.26069233
H	-2.1818094791	-2.5398850304	-0.6215802491
C	-0.9512454192	-3.7351372077	0.6951355203
H	-0.5142292464	-2.7008545912	-1.1465708568
H	-1.5805025967	-3.5912259365	1.5840547006
H	0.0867064354	-3.7385427054	1.056055838
C	-1.2744169165	-5.0853464467	0.0494854735
H	-1.127140382	-5.9136362666	0.7501903567
H	-0.6353726209	-5.2675709419	-0.8221940792
H	-2.3150530945	-5.1187369866	-0.2930875404
C	-2.7295075417	2.8503133547	0.1288001721
H	-1.5639110286	2.3774082862	-1.6382460187
H	-0.7287304129	3.379775424	-0.4607488702
H	-2.5523376568	2.9834105142	1.2055954688
C	-3.8407438987	1.8148666892	-0.07407484
H	-3.0763304634	3.8240384655	-0.2443305102
C	-5.1598902943	2.2270237399	0.5856719748
H	-3.5153620527	0.8472635699	0.3250293396
H	-3.9978234388	1.6616512697	-1.1510165011
H	-5.5273857401	3.1763596651	0.1791948981
H	-5.0342330935	2.359196957	1.6665672149
H	-5.9394857235	1.4739057345	0.4310290688
C	3.1599117039	0.2559547726	0.6218337931
C	4.3551803879	1.2135842362	0.4070114069
H	4.8143145046	1.0469710912	-0.5730106893

H	4.0392292997	2.2600498871	0.4531486714
H	5.1217955391	1.0570640702	1.1749667674
C	2.5494334198	0.5148985844	2.0185212983
H	3.301276812	0.3498689236	2.7986664451
H	2.1864414254	1.5411523172	2.1244895945
H	1.7088840321	-0.1595393429	2.2101993475
C	3.6925145773	-1.1884761179	0.5986177687
H	2.8980023344	-1.9172473679	0.7911978236
H	4.1576437686	-1.4339828373	-0.3615431195
H	4.4529670424	-1.3151065175	1.3761022911
H	4.4529670424	-1.3151065175	1.3761022911

TS exo 0155

E(RB3LYP) = -706.414387883 A.U.

First frequency = -484.5623 cm^{-1}

H	1.123958024	-1.0157638463	-3.1732813957
C	1.1440016449	-0.1858538692	-2.4720500479
H	0.718553252	0.7336744073	-2.8561147398
C	2.0766799541	-0.1869300759	-1.4491939173
C	2.0699444024	0.7718585137	-0.4100617914
C	1.1413099211	1.8008872809	-0.4875449548
H	1.0272538976	2.5083851067	0.3281533588
H	0.8360568089	2.1892283238	-1.4505440292
C	-0.8926436511	0.7754476518	-0.5216683845
H	-0.7960277201	0.6843372672	0.556918252
C	-1.7218886861	1.9380471897	-1.0216921869
C	-0.7761206172	-0.3932462603	-1.27088525
H	-1.3097366765	-0.4344166156	-2.2195298833
C	-0.5116175162	-1.7168639037	-0.5906578526
H	2.675377943	-1.0831468946	-1.3284683783
H	0.3245517474	-1.590857646	0.1102433833
H	-0.1830907695	-2.4553409657	-1.3294363166
C	-1.7296581948	-2.2552857013	0.1828096613
H	-2.0543635363	-1.4901933877	0.8988537941
C	-1.4616448476	-3.5674222193	0.9363257709
H	-2.5692483343	-2.3966338523	-0.5124537466
H	-2.3359575247	-3.8024393699	1.5567828854

H	-0.6254610126	-3.415705278	1.6331949706
C	-1.1582797351	-4.7645233078	0.0278921544
H	-1.9704891045	-4.9259556347	-0.690643505
H	-1.0410294024	-5.6841550225	0.6104800689
H	-0.2360915378	-4.6186371761	-0.5434274172
C	-3.2384399668	1.7471126066	-0.8040742417
H	-1.5403097324	2.0732112787	-2.0967617957
H	-1.4025907383	2.869904624	-0.5411981717
H	-3.7622091887	2.6270720553	-1.2033326436
C	-3.6586759608	1.5341698916	0.6589483479
H	-3.5718390042	0.8861470999	-1.3971905186
C	-3.2440652171	2.6698788742	1.6006240095
H	-3.2388038795	0.5884413817	1.0227499549
H	-4.7488380132	1.4143349099	0.6937152515
H	-2.1547603121	2.7485515786	1.6831688285
H	-3.6383251137	2.5114989023	2.6096023099
H	-3.6181617005	3.6365790318	1.2433727356
C	2.8855555265	0.5803638682	0.8863182954
C	1.9269213398	0.4240693138	2.0896671869
H	2.4958357408	0.3038465502	3.0187352279
H	1.2771280899	1.295640005	2.2108995576
H	1.2870265325	-0.4561026901	1.9681390399
C	3.7941229224	-0.6618073161	0.8376299162
H	4.3822687066	-0.7259358244	1.7589209347
H	3.215219528	-1.5871286298	0.7517538866
H	4.4957170695	-0.6167896915	-0.0017079009
C	3.7822545917	1.8201786476	1.1087546119
H	3.1880802243	2.7347908263	1.1925085234
H	4.3689580242	1.7140527673	2.0286629059
H	4.477931251	1.9502338795	0.273231399
H	4.477931251	1.9502338795	0.273231399

TS exo 0158

E(RB3LYP) = -706.414407747 A.U.

First frequency = -511.6328 cm^{-1}

H	0.5411822329	-1.2784869954	-2.7466484131
C	0.737790738	-0.3930295534	-2.1497680543

H	0.3919335191	0.5282198202	-2.6042138281
C	1.7916809933	-0.4003660874	-1.2507576832
C	2.0414096199	0.6669637532	-0.3580771628
C	1.2401346293	1.7963494757	-0.4705219441
H	1.3133958753	2.6131999808	0.237520478
H	0.8778235261	2.0966530693	-1.445229619
C	-0.9019343164	1.0933556937	-0.2098961769
H	-0.7384340318	1.1605122921	0.8622524546
C	-1.6089309595	2.2674304455	-0.8535187974
C	-1.0158997154	-0.1873783846	-0.7529906738
H	-1.6556775235	-0.3081316182	-1.6265703004
C	-0.8750734218	-1.3918034188	0.1515430538
H	2.2979136559	-1.3475632666	-1.0792762897
H	-1.6781631231	-1.3554086979	0.9043576435
H	0.0609316061	-1.2953344761	0.7154096919
C	-0.9188541136	-2.7571799789	-0.5381070425
H	-1.8320834608	-2.8328462995	-1.1460182743
C	-0.8686290308	-3.9266094011	0.4513245925
H	-0.0787092559	-2.8441863135	-1.2368786002
H	-1.7135267338	-3.8501683899	1.1492418807
H	0.0392012766	-3.8385733537	1.0640804885
C	-0.8926749439	-5.2940268501	-0.2371718527
H	-0.8545590469	-6.1125663725	0.488992498
H	-0.0386690476	-5.4086286772	-0.914667101
H	-1.8040336437	-5.418624981	-0.8332787846
C	-3.1280217263	2.29318326	-0.5886532087
H	-1.4438906265	2.2344166808	-1.9396765255
H	-1.1716534601	3.2115053191	-0.5040186773
H	-3.5730374376	3.1279276436	-1.1483526634
C	-3.499617457	2.4286876303	0.8925005626
H	-3.5766827592	1.3748337929	-0.9908834828
C	-5.0120254017	2.5020302598	1.1200520118
H	-3.0192038468	3.3272542124	1.3043367805
H	-3.0866904837	1.578801302	1.4500796265
H	-5.2558764057	2.5959317954	2.1833529287
H	-5.5099908842	1.6017907966	0.741859463
H	-5.4487364884	3.3623649254	0.5998758762
C	3.0494378824	0.4663197009	0.7921538425

C	2.6295269663	-0.7108738358	1.7026288824
H	3.3740366281	-0.871012583	2.4911352072
H	1.6682335612	-0.5055161776	2.1846760414
H	2.5323067062	-1.6452911206	1.1425714458
C	4.4357767688	0.1611587559	0.1779647809
H	4.4184822213	-0.7473518071	-0.4310419314
H	4.7666367817	0.9854152388	-0.4620226356
H	5.1821445714	0.0197268213	0.9682101883
C	3.1835077629	1.7210535576	1.6742924044
H	3.9360172165	1.5510111916	2.4513673005
H	3.4958043289	2.5926619377	1.0903689989
H	2.2418798629	1.9655179817	2.1770350317
H	2.2418798629	1.9655179817	2.1770350317

TS exo 0166

E(RB3LYP) = -706.414751802 A.U.

First frequency = -492.1542 cm⁻¹

H	0.4423527018	-1.4196184369	-2.7809979252
C	0.6861276914	-0.5271818837	-2.2124157509
H	0.3458855857	0.394944933	-2.667750992
C	1.7441529094	-0.5575362006	-1.3212056989
C	2.0427176655	0.5200714822	-0.4565076263
C	1.3011339531	1.6871864412	-0.6044562791
H	1.4302415273	2.5152237562	0.0860000635
H	0.9600723593	1.9885634469	-1.5865933145
C	-0.8566382519	1.1103863147	-0.2705016628
H	-0.661218771	1.2438440288	0.7900311304
C	-1.5329280352	2.2664762877	-0.9769570259
C	-1.0347051744	-0.1969448753	-0.7175881057
H	-1.697695989	-0.365377446	-1.5645412253
C	-0.8405051095	-1.3448154924	0.2447012199
H	2.2069678351	-1.5212878403	-1.1376088189
H	-1.539861294	-1.2244173826	1.0866309375
H	0.1638461066	-1.2599000891	0.6840479689
C	-1.0215780685	-2.7424874404	-0.3500272792
H	-2.020094359	-2.8204924303	-0.8037419759
C	-0.8428476503	-3.8603784349	0.6826274122

H	-0.3034816957	-2.8880027484	-1.1657689898
H	-1.5606135474	-3.718011619	1.5020131428
H	0.1547491617	-3.7731941778	1.1352188967
C	-1.0148504879	-5.2597980532	0.0856513294
H	-2.0144410263	-5.3830376319	-0.3468150907
H	-0.8796780504	-6.0405755512	0.8412045031
H	-0.2865005357	-5.4387309477	-0.7136584974
C	-3.0411842366	2.376032974	-0.675239699
H	-1.3995472208	2.1519252091	-2.0617411258
H	-1.0469298834	3.2121838678	-0.7048482095
H	-3.4676812559	3.1873373109	-1.2817934664
C	-3.3637783714	2.6321368037	0.8014790655
H	-3.538419906	1.4515581	-0.9984334155
C	-4.864658362	2.7870425419	1.0621444176
H	-2.834928987	3.5360059776	1.1349156868
H	-2.9706280174	1.8068221764	1.4080633258
H	-5.4102523545	1.8847563691	0.7627783436
H	-5.2801171446	3.6265342045	0.4928254097
H	-5.0735369102	2.9665656679	2.1218691248
C	3.0063662157	0.3722346549	0.7395922356
C	4.1643252572	1.3841661693	0.5754013697
H	3.7912446914	2.4119500004	0.5366703147
H	4.8672022346	1.3102018313	1.4135165996
H	4.7163466872	1.1948596693	-0.3511264666
C	2.2624278248	0.6657403052	2.0628632837
H	2.9500432608	0.581910748	2.9121268864
H	1.8394163477	1.6741165131	2.081651539
H	1.4438768454	-0.0441128728	2.2186151914
C	3.6135455721	-1.0390799909	0.8414829723
H	4.3060545574	-1.0837353651	1.6883710388
H	2.843943339	-1.8014461951	1.002684674
H	4.176054716	-1.3048507745	-0.0593345815
H	4.176054716	-1.3048507745	-0.0593345815

TS exo 0182

E(RB3LYP) = -706.413399853 A.U.

First frequency = -510.8825 cm^{-1}

H	1.1664763334	-0.4355378731	-3.2893789061
C	1.0208302569	0.2037687316	-2.4221794551
H	0.3856955916	1.0630152199	-2.6114166797
C	2.0083064524	0.2474562678	-1.4479128713
C	1.8422261298	0.9427047765	-0.2286355377
C	0.6843616872	1.6853436362	-0.0568101199
H	0.4635669426	2.1652825995	0.8874327025
H	0.2023530678	2.1443351311	-0.9100083616
C	-1.0774459412	0.1747285639	-0.3821970666
H	-0.9334995502	-0.1086745519	0.6575506859
C	-2.2056919451	1.1459476848	-0.6648988535
C	-0.6504813331	-0.720650301	-1.3644109712
H	-1.2113649767	-0.7184813217	-2.2993004615
C	-0.0540186134	-2.0526954627	-0.9651920887
H	2.8246391332	-0.4660302103	-1.5286442615
H	0.7030382304	-1.8822053236	-0.1911512322
H	0.4731159991	-2.5033964135	-1.815288711
C	-1.1003182496	-3.046953987	-0.4341652841
H	-1.6181624378	-2.6002779131	0.4253923637
C	-0.4933372266	-4.3934505346	-0.0243500198
H	-1.8721490092	-3.21101839	-1.1995954876
H	0.2806917673	-4.2219661723	0.7363722464
H	0.0232985172	-4.8353706646	-0.8873481895
C	-1.533397103	-5.3805550956	0.513026681
H	-2.3011861175	-5.5921372075	-0.2400376006
H	-2.0415629994	-4.975063326	1.3954815677
H	-1.0758874273	-6.3331499134	0.7998006734
C	-2.572068619	2.077096531	0.4957163761
H	-3.1033935506	0.5708732395	-0.9399963259
H	-1.965716637	1.7451249111	-1.5570589766
H	-2.7662258084	1.4719572192	1.3928737985
C	-3.7952349068	2.9522071368	0.2014115025
H	-1.7214449703	2.7225623958	0.7431415858
C	-4.1558331894	3.883722591	1.3620358935
H	-4.6535565069	2.3088201664	-0.035549935
H	-3.6037318635	3.547214253	-0.7021624558
H	-4.3807206166	3.3124088806	2.2699837563
H	-5.0315737853	4.4980195132	1.1289397214

H	-3.326045288	4.5604325999	1.5962855766
C	2.847816987	0.6970905433	0.9160010587
C	2.8449466379	-0.7909133275	1.3366874296
H	3.5804369396	-0.9679528868	2.1300443297
H	1.8611774921	-1.0840030414	1.7182141966
H	3.091280681	-1.4510217229	0.5003424797
C	4.2616467822	1.0839575359	0.4239126697
H	4.9999457892	0.9249088879	1.2183075755
H	4.5693778398	0.488212841	-0.4401907559
H	4.2956156912	2.1383726385	0.1313523596
C	2.5303375448	1.541846289	2.1636149775
H	1.5611024758	1.2759509089	2.5982100639
H	3.2917313521	1.3711111677	2.9318271642
H	2.5199914505	2.6119691487	1.9333813267
H	2.5199914505	2.6119691487	1.9333813267

TS exo 0185

E(RB3LYP) = -706.413290488 A.U.

First frequency = -520.0538 cm⁻¹

H	0.1774939918	-0.2204412596	-3.0547942368
C	0.3638981606	0.3715938914	-2.1625528639
H	-0.2438408746	1.2648399947	-2.0889793289
C	1.6042852014	0.2941284316	-1.5482550477
C	1.8794822583	0.9042601632	-0.3038146652
C	0.8729589768	1.6653286651	0.2755649909
H	0.9820936193	2.0802606279	1.2703294342
H	0.1904696523	2.2191857762	-0.3557767089
C	-0.8927526261	0.2689722579	0.5283376957
H	-0.3771808308	-0.1636655354	1.3830467715
C	-1.9501816411	1.2941437501	0.9021605587
C	-0.9672894832	-0.5322738595	-0.614649935
H	-1.8129261714	-0.3854269063	-1.2825221234
C	-0.4031290061	-1.9365504706	-0.5788686726
H	2.2999984908	-0.4551691009	-1.9182598394
H	0.601665403	-1.9044004723	-0.1409911031
H	-0.2815902409	-2.3253240729	-1.5974626236
C	-1.2723730526	-2.9121470559	0.2329329045

H	-1.3840459643	-2.5291666666	1.2564859715
C	-0.6987604449	-4.3328863733	0.2771711238
H	-2.286194222	-2.9394279786	-0.1912462896
H	0.3157697701	-4.2977612569	0.6975554966
H	-0.5883672682	-4.7108613454	-0.7484636578
C	-1.5603285094	-5.3016671659	1.0920828475
H	-2.5703861002	-5.3777487463	0.6732964992
H	-1.6595085986	-4.9626120226	2.1296790223
H	-1.1298167388	-6.3083372162	1.1097731584
C	-2.6547047295	2.0029999704	-0.2614856445
H	-1.5094115238	2.0540159057	1.5609496946
H	-2.71534054	0.7896711972	1.5132291059
H	-1.9132294357	2.4810927542	-0.9156574172
C	-3.6584899149	3.0612463265	0.2103148012
H	-3.1797363778	1.2682466784	-0.8852116188
C	-4.3768213268	3.7602320634	-0.9472144828
H	-3.1355766994	3.8070580519	0.8242056332
H	-4.3972839247	2.5880049149	0.8713774741
H	-4.9346505412	3.0403645766	-1.5570401408
H	-3.6618995237	4.2658349541	-1.6064830187
H	-5.0862087953	4.5117120376	-0.5858505607
C	3.1693445995	0.5198784576	0.4497258851
C	3.3203970798	1.2878723693	1.7758181848
H	2.5219227354	1.0394456676	2.4826924197
H	4.2713298835	1.0259353634	2.2514047034
H	3.3111710511	2.3708750675	1.6165446864
C	3.1808137969	-0.9929469736	0.7714823139
H	3.1152111882	-1.6014889419	-0.1347962437
H	4.1044544209	-1.2691542656	1.2933959836
H	2.3365566128	-1.2587084043	1.4163718982
C	4.3860006878	0.8603126567	-0.4412712816
H	4.4113024065	1.9303820214	-0.6712095341
H	5.3195875556	0.5975245947	0.0694093275
H	4.3612285891	0.3162276072	-1.3897467855
H	4.3612285891	0.3162276072	-1.3897467855

TS_{exo} 0190

E(RB3LYP) = -706.414388044 A.U.

First frequency = $-492.8494 \text{ cm}^{-1}$

H	0.5112079969	-1.2937340855	-2.6003444426
C	0.7530300691	-0.3946502577	-2.041248828
H	0.2810609857	0.5037760092	-2.4193053145
C	1.9172550015	-0.3522737374	-1.2945911932
C	2.2357182341	0.726158659	-0.4383860334
C	1.3792529247	1.8226263477	-0.4418737919
H	1.5295580379	2.6426700584	0.2540009148
H	0.886331298	2.1163652301	-1.3599561725
C	-0.6436788252	1.0665121243	0.1637818214
H	-0.3280283869	1.1678936778	1.200610801
C	-1.5076134306	2.1947401571	-0.3588163204
C	-0.7831704304	-0.2322091406	-0.3241548177
H	-1.5282095886	-0.4043702849	-1.0956205956
C	-0.3900799739	-1.4036246207	0.5473567854
H	2.4803644591	-1.2752549275	-1.2061197029
H	-0.9207000656	-1.3269403578	1.5090745566
H	0.6762068886	-1.3037622359	0.792726643
C	-0.6571551495	-2.7903183931	-0.0492455652
H	-0.1376836929	-2.8806697779	-1.0114395237
C	-2.1456202176	-3.1101189001	-0.2419515669
H	-0.2167817007	-3.5513280646	0.6087220121
H	-2.6057298941	-2.3641945205	-0.9023250278
H	-2.6600586792	-3.0153519538	0.7243449849
C	-2.3819637862	-4.5092557582	-0.8176099878
H	-3.4491467892	-4.7196948084	-0.9426628573
H	-1.9636494458	-5.2812159213	-0.1614505171
H	-1.9032948714	-4.6168061647	-1.7978196854
C	-2.8629247404	2.3200980955	0.3694978738
H	-1.6887281455	2.0454571788	-1.432980141
H	-0.9815936409	3.1527262514	-0.2654546204
H	-2.6788222181	2.4714591516	1.4426974203
C	-3.8098654423	1.129033585	0.184880472
H	-3.3640977132	3.2320304698	0.0160689642
C	-5.1605511766	1.3360914479	0.8762748512
H	-3.3348061244	0.2197748927	0.570481692
H	-3.9669522971	0.9567801773	-0.8892596747

H	-5.6766329774	2.2197651857	0.4834979161
H	-5.0313407002	1.4834296837	1.9547933569
H	-5.8205174315	0.4739054749	0.7350975193
C	3.359444417	0.637781454	0.6150371847
C	4.1193251063	-0.7001205915	0.5607440706
H	4.5747819522	-0.8677327718	-0.4206290688
H	4.9240520774	-0.6989630257	1.303185804
H	3.4647263505	-1.5489169352	0.7845670618
C	4.3746106724	1.7768234575	0.362315708
H	4.8167117666	1.6878774015	-0.6355046626
H	3.8968228006	2.7587651545	0.4284514694
H	5.1853545738	1.745055673	1.0995803709
C	2.7675393555	0.7927596466	2.034961028
H	2.0543183233	-0.0089678708	2.2513252067
H	3.564084424	0.7508488923	2.7866118022
H	2.2471582347	1.7466229238	2.160227327
H	2.2471582347	1.7466229238	2.160227327

TS exo 0194

E(RB3LYP) = -706.413845627 A.U.

First frequency = -511.8648 cm⁻¹

H	0.0455516221	-1.0791571304	-2.637755706
C	0.3225025386	-0.2583677395	-1.9831094208
H	-0.149177798	0.6839092388	-2.2362476745
C	1.5357928756	-0.3003779657	-1.3165085567
C	1.9157978404	0.6682044647	-0.3595367538
C	1.0584014603	1.7441368971	-0.1635048106
H	1.2401350039	2.4754457304	0.6151091057
H	0.4941531384	2.1328238121	-1.0015821376
C	-0.9469321251	0.8811328337	0.42386691
H	-0.5839012568	0.8331689405	1.4483526202
C	-1.823668101	2.0689487521	0.0952947397
C	-1.1181192564	-0.33266257	-0.2440315327
H	-1.9163026111	-0.3916949073	-0.9831368252
C	-0.7421872048	-1.6223719862	0.4505307085
H	2.1063839853	-1.2246502663	-1.3719901872
H	-1.3678201722	-1.7267151743	1.3508870018

H	0.2877888967	-1.53189666	0.8172533803
C	-0.8781716595	-2.8972126356	-0.3849837259
H	-1.8963793391	-2.9606495986	-0.7954833948
C	-0.5719900882	-4.1691152074	0.4134562395
H	-0.2037182277	-2.8459219139	-1.2476364499
H	-1.2505319359	-4.2308204432	1.2751734373
H	0.4416734008	-4.0945732479	0.8309505568
C	-0.6891719667	-5.4446468677	-0.4254400232
H	-0.4646707717	-6.3386886388	0.1653902009
H	0.0040185195	-5.4225698486	-1.2742459958
H	-1.7013288684	-5.5576906	-0.8306739147
C	-3.2079706102	1.9799496792	0.7656149148
H	-1.9458983275	2.132722513	-0.9942066949
H	-1.3408457734	3.0045328123	0.4069350893
H	-3.7179607823	1.0746520896	0.4094437756
C	-4.1040520973	3.2047994741	0.5265531962
H	-3.0647535716	1.8432975097	1.8457155866
C	-4.5045708532	3.4091461676	-0.9391502709
H	-3.5919433813	4.1043320539	0.8952300667
H	-5.0118207846	3.1009405799	1.1345495521
H	-3.6363071919	3.6141589104	-1.573563992
H	-5.1955252701	4.2514851588	-1.0475025801
H	-5.0014496731	2.5164876639	-1.3371084717
C	3.1467635007	0.404140213	0.5317086927
C	4.3893879811	0.2744818124	-0.3801775465
H	4.5430365235	1.190715091	-0.9592801287
H	5.2883460203	0.0935771072	0.2204369707
H	4.2884572285	-0.5537955517	-1.0875611499
C	3.4019393113	1.5510073956	1.5266721814
H	2.5731650465	1.6664472356	2.23305963
H	4.3046495106	1.3432281923	2.1106083294
H	3.5482573335	2.5059455155	1.0119923292
C	2.978259917	-0.900328576	1.3447816819
H	2.8098716793	-1.765585051	0.6973556117
H	3.8762860602	-1.1001620882	1.9408860693
H	2.129196143	-0.8231518764	2.0316331244
H	2.129196143	-0.8231518764	2.0316331244

TS exo 0198

E(RB3LYP) = -706.414105297 A.U.

First frequency = -487.2700 cm⁻¹

H	0.34791399	-1.6281671555	-2.4331240662
C	0.5931639737	-0.6940349855	-1.9366183555
H	0.0644121245	0.1675503267	-2.325359816
C	1.7993931862	-0.5741898761	-1.2703978261
C	2.1350001736	0.5605047217	-0.4965363287
C	1.2449575475	1.6285113608	-0.5022773299
H	1.4102733962	2.489473951	0.1384169431
H	0.6773155675	1.8536813794	-1.3960089847
C	-0.7191703046	0.8254248103	0.2711668486
H	-0.3392975411	1.0016319262	1.2753340103
C	-1.651515873	1.8859679557	-0.2707999998
C	-0.8401012956	-0.501301366	-0.1348727386
H	-1.6302857997	-0.741952546	-0.841655238
C	-0.345872713	-1.6040814813	0.7736301952
H	2.3983419491	-1.4730687896	-1.169940461
H	-0.9179503037	-1.5645119084	1.7139109089
H	0.6915074491	-1.3715682432	1.0503863252
C	-0.414377714	-3.0339404478	0.2232316101
H	0.2195624724	-3.116404642	-0.6676338443
C	-1.8299874648	-3.5177444424	-0.1157831105
H	0.0191075064	-3.7137876544	0.969239341
H	-2.2658592966	-2.8790281222	-0.8942301941
H	-2.4725366952	-3.4015706094	0.7678720803
C	-1.8584232919	-4.9744558142	-0.5876871903
H	-2.8753481707	-5.3019532698	-0.8273189384
H	-1.4636138969	-5.6462879844	0.1831248974
H	-1.244267137	-5.1083382187	-1.4857289371
C	-3.0279307932	1.874000706	0.4174644514
H	-1.7915799607	1.7323243015	-1.3507626063
H	-1.2071168257	2.8832213113	-0.1580616699
H	-3.4861826691	0.8849394625	0.2838497985
C	-3.9766830665	2.95789135	-0.105976599
H	-2.8906028005	1.9999992099	1.5006624022
C	-5.3446536426	2.936830191	0.582065025

H	-4.1068350249	2.8309380835	-1.1895275648
H	-3.5105507117	3.9433696809	0.0299383193
H	-5.2443051717	3.0933779329	1.6622015278
H	-5.8445187332	1.9726638795	0.43457835
H	-6.0047388818	3.7182314276	0.1915140745
C	3.3315195084	0.5675196901	0.4777878529
C	4.2954818298	1.7085238363	0.0764827871
H	4.6673203614	1.5614120416	-0.9428812656
H	3.7968692656	2.681707897	0.1117777679
H	5.1574263008	1.7450026448	0.7529883459
C	2.8399914118	0.8065154524	1.9239997086
H	3.6901045257	0.8344175336	2.6151526486
H	2.3040563323	1.7546235898	2.024110128
H	2.1672338343	0.0056249341	2.2469113324
C	4.1205460316	-0.7544792905	0.4578061064
H	4.9721239397	-0.6875085924	1.1427494122
H	3.503810025	-1.6005974141	0.7784328002
H	4.5150284732	-0.9760201433	-0.5391358877
H	4.5150284732	-0.9760201433	-0.5391358877

TS exo 0204

E(RB3LYP) = -706.413555399 A.U.

First frequency = -513.2362 cm^{-1}

H	0.4868125888	-0.9076113888	-2.9189042094
C	0.6769698694	-0.1357989397	-2.1792206236
H	0.2218787033	0.8192747128	-2.4138787215
C	1.8091273364	-0.2196062866	-1.3859338611
C	2.0679122902	0.6793247707	-0.3261178527
C	1.1792642533	1.7339700413	-0.1516301885
H	1.2652479582	2.4094557634	0.6912296877
H	0.709637757	2.1801431875	-1.0190393584
C	-0.8617003775	0.8272656815	0.1506545714
H	-0.6139331305	0.7084954874	1.2033726696
C	-1.7112915675	2.0323088138	-0.1873910431
C	-0.9477145217	-0.3383768933	-0.6128749558
H	-1.6589454284	-0.3485761801	-1.4379411419
C	-0.6321748177	-1.6716105377	0.0280517123

H	2.3959129288	-1.1334900854	-1.4443007211
H	-1.3146549412	-1.8111769179	0.8784428134
H	0.3743558187	-1.6197715102	0.4620676272
C	-0.7267528578	-2.8864271249	-0.8994652132
H	-1.7399002033	-2.9421747533	-1.3236611407
C	-0.3873440877	-4.2207854192	-0.217150784
H	-0.0475235342	-2.7415528014	-1.7464072155
H	0.6262923783	-4.1594125947	0.2029638229
H	-0.3523057736	-5.0079337356	-0.9811029448
C	-1.3711701754	-4.6381016087	0.8821017454
H	-1.1186018331	-5.6240535256	1.2858740055
H	-2.3945957773	-4.6892806301	0.4921369366
H	-1.3716618586	-3.9318611666	1.7183224438
C	-3.162462651	1.8944639594	0.3060814006
H	-1.7185869908	2.1797111282	-1.2773154009
H	-1.2760067477	2.9437306902	0.2422852639
H	-3.6098749654	0.9975514665	-0.1427587112
C	-4.0289010136	3.118056622	-0.0121505622
H	-3.1595383467	1.7205326692	1.3913469304
C	-5.4720907797	2.9717794399	0.4787357307
H	-4.0241952424	3.2911100455	-1.097124653
H	-3.5744287519	4.0106360639	0.4391354321
H	-5.9584405627	2.104327674	0.0180556073
H	-6.0711782218	3.8564643617	0.2394355288
H	-5.5058164819	2.8293330789	1.5649398655
C	3.1957384597	0.3590570897	0.6763119028
C	4.5337492651	0.3021003177	-0.0975936858
H	4.5233339937	-0.4739239895	-0.8684998145
H	4.7384885069	1.2583328663	-0.5896860676
H	5.3626668155	0.0836167384	0.5856091163
C	3.3229644267	1.43318291	1.7720428797
H	4.1580579902	1.1893216473	2.4370068553
H	3.5123419707	2.4234387072	1.3457323897
H	2.4194164331	1.4928286733	2.3878664189
C	2.9557378951	-1.0011420919	1.3714861265
H	2.8763621039	-1.8192714718	0.6499948194
H	3.7826606792	-1.236118365	2.0517145201
H	2.0323172472	-0.979503048	1.9591675263

H 2.0323172472 -0.979503048 1.9591675263

TS exo 0207

E(RB3LYP) = -706.413430946 A.U.

First frequency = -493.9355 cm⁻¹

H 1.1023180747 -0.3443701047 -3.3954375106
C 0.9810815307 0.2610184931 -2.5008219303
H 0.3271697231 1.1163964553 -2.6298188507
C 1.9798590955 0.2481111602 -1.5399837202
C 1.8364756978 0.889941552 -0.2889944971
C 0.699004788 1.6543418452 -0.074739205
H 0.5077499225 2.0912957383 0.8993163723
H 0.2212731036 2.173500322 -0.8951934543
C -1.0959948476 0.1889447451 -0.4079617005
H -0.9438532433 -0.0900736476 0.6316358924
C -2.2074567071 1.1810957297 -0.684137693
C -0.688080691 -0.7124388161 -1.3877360223
H -1.2472941148 -0.7156206205 -2.3226308348
C -0.0450791264 -2.0216658168 -0.9910025038
H 2.7828316137 -0.468578057 -1.6721189569
H 0.7513076848 -1.8144842263 -0.2644657368
H 0.4452848964 -2.481560091 -1.8577598856
C -1.0348645441 -3.0253433396 -0.3754718605
H -1.5194835772 -2.5658150963 0.4964098373
C -0.3696115838 -4.3414244096 0.0424635722
H -1.8403114919 -3.2336518886 -1.0938079516
H 0.4371393743 -4.1249917491 0.7564800339
H 0.1147202688 -4.7964637307 -0.8323587556
C -1.3520175727 -5.3385582439 0.663237544
H -1.8256781669 -4.9188586445 1.5581382203
H -0.8532276655 -6.2687110278 0.9547621085
H -2.1509361594 -5.5948638097 -0.0420045079
C -2.5548417288 2.1086041091 0.4851972112
H -3.1152726779 0.6247911021 -0.9638189153
H -1.9563447405 1.7838758024 -1.5706670058
H -2.7661059556 1.4989046296 1.3753623926
C -3.7552425286 3.0166007603 0.1973020324

H	-1.6888795428	2.7300573024	0.7415782601
C	-4.097154865	3.9430610493	1.3675822005
H	-4.6280754053	2.3970186041	-0.0498593803
H	-3.5462381552	3.617161749	-0.6986788509
H	-3.2519754616	4.5965815957	1.6124271836
H	-4.339121172	3.3668721746	2.2680246451
H	-4.9568352597	4.5812004658	1.1388349372
C	2.7924288464	0.6069464457	0.8904703822
C	3.9361405684	-0.3515417094	0.5109717886
H	4.6016666477	-0.4910105929	1.3691462786
H	3.5605387196	-1.3382120173	0.2207670825
H	4.5380898679	0.042845826	-0.3141312111
C	3.4202619919	1.9393401973	1.3611802773
H	4.1021364624	1.7708912635	2.2028849756
H	3.9877948598	2.4080921204	0.5504956955
H	2.6541042813	2.6498048085	1.685079645
C	2.009313997	-0.0272236823	2.0632950594
H	2.6774597366	-0.2124726621	2.9121381073
H	1.2012855878	0.6207212646	2.4145485954
H	1.5662855842	-0.9835420441	1.7666867906
H	1.5662855842	-0.9835420441	1.7666867906

TS exo 0214

E(RB3LYP) = -706.412867568 A.U.

First frequency = -516.2878 cm^{-1}

H	1.3134016232	-0.5002914356	-3.3470422977
C	1.1436403941	0.1291887829	-2.4769444841
H	0.4542090361	0.9480228822	-2.6560192167
C	2.1458623637	0.2375539763	-1.5220021786
C	1.9576290753	0.924119569	-0.3020393513
C	0.7570827147	1.5914834531	-0.1118590881
H	0.5220912326	2.0578187428	0.8358373438
H	0.234993081	2.020593711	-0.9571480773
C	-0.8981189439	-0.031261939	-0.4041702982
H	-0.7150707186	-0.3001110708	0.6320416081
C	-2.0944111381	0.8617825531	-0.6667750159
C	-0.4369793979	-0.9031027518	-1.3943406386

H	-1.0173629441	-0.9329781558	-2.3175895236
C	0.2392093106	-2.207784164	-1.0254726537
H	3.0032663295	-0.4240372327	-1.6169632655
H	0.885315947	-2.0393720821	-0.1560329566
H	0.9000430106	-2.5297883797	-1.8384989416
C	-0.7437994824	-3.3562934583	-0.7171522703
H	-1.3973659436	-3.5153178637	-1.5870207722
C	-1.6100616523	-3.1583148049	0.5319342051
H	-0.1645860961	-4.2833007688	-0.6017122027
H	-2.2351682664	-2.2666710696	0.4077781408
H	-0.9583709736	-2.9545297886	1.3932179636
C	-2.4978490714	-4.3695132201	0.8325387102
H	-3.175213597	-4.5774201186	-0.0039040815
H	-3.1112691779	-4.2077778503	1.7250564826
H	-1.8962729125	-5.2704851546	0.9995077732
C	-2.5102228507	1.7536329975	0.5077770135
H	-2.9538212327	0.2290425803	-0.9377248971
H	-1.9072007875	1.4843873242	-1.5555784796
H	-2.6547796809	1.1264206158	1.3991395969
C	-3.7915943401	2.5486535875	0.2351545213
H	-1.7014833694	2.4509602226	0.755154298
C	-4.2030696377	3.4392840329	1.4108442099
H	-4.6071560072	1.8522589301	-0.0030441461
H	-3.6485553726	3.1663400118	-0.6621411872
H	-4.3810167008	2.8427858164	2.3129850969
H	-5.1199813588	3.9964608494	1.1930436891
H	-3.4182675937	4.1670126194	1.647151577
C	2.9897825284	0.7359514432	0.8292718509
C	4.3774744402	1.1854239003	0.3169239478
H	5.1319835132	1.0663935188	1.1030074887
H	4.7029328975	0.5993258821	-0.5472202798
H	4.3582949864	2.2383773514	0.0177911823
C	2.6491548655	1.5729043194	2.07610233
H	2.5804652398	2.6392807382	1.8384715612
H	1.7017659024	1.2614080538	2.5281302486
H	3.4300690994	1.4468919592	2.8333042165
C	3.0601439757	-0.7483543245	1.2570412555
H	2.0959535135	-1.0829211054	1.6541650448

H	3.3224682152	-1.4007343877	0.4195376625
H	3.8141939516	-0.8883659832	2.0403349726
H	3.8141939516	-0.8883659832	2.0403349726

TS exo 0218

E(RB3LYP) = -706.413107392 A.U.

First frequency = -488.0493 cm⁻¹

H	1.1541411232	-0.7771022358	-3.3043103074
C	1.204556911	0.0006461782	-2.5468787828
H	0.7941399088	0.9536912093	-2.8601015264
C	2.1654519328	-0.0871169815	-1.5527128732
C	2.2014212938	0.7964447094	-0.4500373134
C	1.2954279805	1.8481874426	-0.4350365373
H	1.2134779803	2.4984753678	0.430518002
H	0.9789962516	2.3085952193	-1.361739735
C	-0.7743669585	0.8640534559	-0.5145611398
H	-0.6575746046	0.7147978491	0.553516507
C	-1.5669596316	2.0747544624	-0.9622556932
C	-0.6768737366	-0.2607137569	-1.3317045532
H	-1.2323285986	-0.244955052	-2.2686533122
C	-0.4189699643	-1.62291785	-0.7293422474
H	2.7498764941	-0.9996819545	-1.5104791645
H	0.4388895474	-1.5482661368	-0.0481490584
H	-0.125632464	-2.333478476	-1.5118513223
C	-1.6221548827	-2.1864314413	0.0453215776
H	-1.8926427732	-1.4874102001	0.8463472492
C	-1.3562421583	-3.5710929661	0.6457173108
H	-2.4959802429	-2.236640691	-0.6198482465
H	-0.4757806646	-3.5154122674	1.3008483948
H	-1.0917984427	-4.2717094569	-0.1580843915
C	-2.5499271687	-4.1175453533	1.434057577
H	-2.8130883482	-3.4490660744	2.2618717446
H	-2.3377262728	-5.1051175764	1.8566825957
H	-3.434499655	-4.2113466257	0.7936483164
C	-3.1064664695	1.9352396416	-0.891663862
H	-1.299347045	2.2843436245	-2.0076626666
H	-1.2674689889	2.962289233	-0.3902136637

H	-3.539290839	2.695750276	-1.5551759392
C	-3.7411532497	2.1140616656	0.4973669599
H	-3.3970757399	0.9615044984	-1.3078106725
C	-3.4696272947	0.9917509322	1.5051629425
H	-4.8271829013	2.2047886047	0.3639827387
H	-3.4095616322	3.0733158582	0.9188575929
H	-3.7510524905	0.0173733995	1.0915836599
H	-4.0450852861	1.1447088649	2.4244921707
H	-2.4140104749	0.9370725038	1.7839963445
C	3.0434457415	0.5002467379	0.8093467794
C	3.9746035873	1.7022159915	1.0902517799
H	4.5814499903	1.5214959234	1.9851241392
H	4.6520674771	1.8728732782	0.2470891938
H	3.4044547542	2.6219386381	1.2504166832
C	2.1111400336	0.2849610622	2.0241752339
H	1.4849855473	1.160348957	2.2194758708
H	1.4483278838	-0.5713534426	1.8617991637
H	2.6998109315	0.0909718986	2.928133408
C	3.9204059566	-0.7558558845	0.6547945373
H	3.3173063165	-1.6597125594	0.5205934993
H	4.6036430365	-0.6696881428	-0.1963768821
H	4.5276801505	-0.895808563	1.5550420352
H	4.5276801505	-0.895808563	1.5550420352

TS exo 0229

E(RB3LYP) = -706.413188042 A.U.

First frequency = -518.6371 cm⁻¹

H	0.4270280774	-0.2946111971	-3.0160750805
C	0.5489991047	0.3111516319	-2.1219883072
H	-0.1594114539	1.1258434731	-2.038480835
C	1.7932078022	0.3766427604	-1.5148574118
C	2.0024770233	1.0078171623	-0.2679270478
C	0.9166830462	1.6405683176	0.3230137889
H	0.9839065047	2.060759806	1.3192859819
H	0.1690012053	2.1137042472	-0.3003231077
C	-0.6655509116	0.0464380852	0.5835691475
H	-0.0957093679	-0.3329716224	1.429089639

C	-1.83123359	0.9379498508	0.9788834676
C	-0.6618569008	-0.746986534	-0.5672701696
H	-1.5200430308	-0.6787558668	-1.2297856407
C	0.056387878	-2.0816881587	-0.5519599402
H	2.5703882997	-0.2827883866	-1.8936506106
H	1.072439806	-1.928961738	-0.1713010856
H	0.1631045445	-2.4631670883	-1.5751421614
C	-0.6454590858	-3.14689839	0.3131621438
H	-0.0293785698	-4.0571686665	0.3271480899
C	-2.0582909398	-3.504575069	-0.1621511161
H	-0.6949701874	-2.7915024607	1.3516405419
H	-2.014277186	-3.8314201635	-1.2105734418
H	-2.6834851595	-2.602660694	-0.1501356282
C	-2.7154802138	-4.5933447548	0.6904947073
H	-2.1273903247	-5.5181965688	0.6720519102
H	-3.7234707519	-4.8317999623	0.3352501477
H	-2.7967252842	-4.2768156203	1.7368280734
C	-2.6370820081	1.5546696205	-0.1712054567
H	-1.4735960968	1.7461173979	1.6305006467
H	-2.5183876336	0.3453919102	1.6033626916
H	-1.9693359296	2.1113475911	-0.8425319453
C	-3.7466763557	2.4920921634	0.318537568
H	-3.0865116493	0.7605860505	-0.7812769271
C	-4.5656029466	3.0958351507	-0.8257071484
H	-3.301094415	3.2971990998	0.9183308913
H	-4.4113488698	1.9402158122	0.997087691
H	-3.9283466551	3.6770562081	-1.5020727631
H	-5.3498334574	3.7619567139	-0.4518353356
H	-5.0485917347	2.3122993029	-1.4207400779
C	3.334114757	0.7754592393	0.4747307348
C	4.4947012971	1.2687215116	-0.4196037743
H	4.5288628366	0.7349191568	-1.3736302327
H	4.3894691276	2.3362706447	-0.6383390617
H	5.4566469086	1.1152700885	0.0829277756
C	3.4001473073	1.5437076688	1.8076235317
H	3.2597064184	2.6191940842	1.6594279857
H	2.6420601397	1.1942151763	2.5162278923
H	4.3788184899	1.3938118477	2.275323333

C	3.5301602266	-0.7278056576	0.7813170099
H	2.725776653	-1.1005885237	1.424119467
H	3.5372397455	-1.3306617212	-0.1310904953
H	4.4818100386	-0.8947333293	1.2992755855
H	4.4818100386	-0.8947333293	1.2992755855

TS_{exo} 0232

E(RB3LYP) = -706.414101987 A.U.

First frequency = -511.2605 cm⁻¹

H	0.2951124864	-1.2215216026	-2.4584043848
C	0.5655182429	-0.3230096318	-1.9117148571
H	0.0706340109	0.573669129	-2.2654216551
C	1.7891007084	-0.2643742942	-1.2655494319
C	2.1633247946	0.8140132041	-0.4318559903
C	1.2827546371	1.8858848582	-0.3405226663
H	1.464367847	2.706930236	0.3428227263
H	0.6955258511	2.1643113817	-1.206569653
C	-0.664297985	1.0673984543	0.4098378386
H	-0.2689636639	1.1052485816	1.4236721354
C	-1.5726446762	2.2189126317	0.0331308637
C	-0.8493004492	-0.2025329798	-0.1427967276
H	-1.6525671537	-0.3151722464	-0.8651408484
C	-0.4644668649	-1.4316197031	0.6537577724
H	2.378364052	-1.1775427077	-1.2243476691
H	-0.9603702623	-1.3858442212	1.6358974246
H	0.6104390947	-1.3849175103	0.8648707068
C	-0.808973457	-2.7764996461	0.0023152259
H	-0.3187765118	-2.8490216148	-0.9765888457
C	-2.3147486129	-3.0230917378	-0.1636449528
H	-0.3867787588	-3.5843493883	0.6148762355
H	-2.7573042284	-2.2356523197	-0.7867471432
H	-2.801266365	-2.9396343636	0.8180599573
C	-2.6274704752	-4.3892747751	-0.7805645577
H	-2.2297512271	-5.2017481345	-0.1615823839
H	-2.1768378663	-4.4835774168	-1.7753499391
H	-3.7056953001	-4.5473070196	-0.8866978088
C	-2.8529636975	2.2903727466	0.8965995758

H	-1.8422801752	2.1375962894	-1.0282000986
H	-1.0458498888	3.1751126335	0.1393181582
H	-2.5526080618	2.4080972112	1.9464672558
C	-3.8061271124	1.0904113338	0.7844855149
H	-3.3996772637	3.2059065186	0.6303300952
C	-4.4291037171	0.9136095668	-0.6042709598
H	-4.6095993278	1.2171255924	1.5211932074
H	-3.274384839	0.1739021359	1.0661737
H	-4.9729689668	1.8151206835	-0.9100042807
H	-5.1348834434	0.0766482189	-0.6172165166
H	-3.6717490581	0.7141713668	-1.3692534305
C	3.407335195	0.6746913453	0.4688981727
C	3.2616117061	-0.5268575082	1.4314615149
H	3.120968392	-1.4667541817	0.8901945981
H	4.1579986206	-0.6322892921	2.0536766824
H	2.4029381026	-0.3895588785	2.0966878383
C	4.6441787435	0.4547017691	-0.4329220854
H	4.5481851235	-0.4507035943	-1.0391915996
H	4.7824986691	1.299743683	-1.1150309431
H	5.5497187373	0.3543465274	0.1765738098
C	3.654226057	1.9343031077	1.319361706
H	2.8327631148	2.1183248258	2.0197106566
H	4.5677163661	1.8109001378	1.9103777106
H	3.7771523643	2.8247472708	0.6946584792
H	3.7771523643	2.8247472708	0.6946584792

TS exo 0245

E(RB3LYP) = -706.414602789 A.U.

First frequency = -492.3621 cm^{-1}

H	-0.0409511609	-0.938948172	-2.8513167791
C	0.2562203684	-0.1908556416	-2.1224812613
H	-0.1848792845	0.7851161785	-2.2836805856
C	1.4393507576	-0.3544875275	-1.4243533749
C	1.8284668848	0.5052970449	-0.3721056907
C	1.0277045103	1.6148211629	-0.1201154799
H	1.2322811037	2.2621226605	0.7274854647
H	0.5308728879	2.1168253421	-0.9406068302

C	-1.0285708322	0.833317864	0.3596998348
H	-0.6927431767	0.7341567389	1.3897648737
C	-1.8528185303	2.0643027384	0.0555099527
C	-1.222752036	-0.3467003698	-0.3553685047
H	-2.0010470288	-0.3668197392	-1.1162357292
C	-0.8234973384	-1.6625092625	0.2673701802
H	1.9594940481	-1.29815885	-1.5496092022
H	-1.3867606928	-1.8008785697	1.2037588062
H	0.2293512943	-1.582375534	0.5669468005
C	-1.0272584953	-2.8968897186	-0.6149862957
H	-2.0770258824	-2.935780664	-0.9362132342
C	-0.6593235029	-4.2198095138	0.0735682627
H	-0.4301259809	-2.7915482389	-1.5286072173
H	-0.9359628076	-5.0512208008	-0.5870599529
H	-1.2642639698	-4.3387122567	0.9829961644
C	0.8275204446	-4.3393605344	0.4306714531
H	1.1287630023	-3.59305165	1.1727219442
H	1.455670461	-4.1939524489	-0.4563412662
H	1.0591880541	-5.3257568575	0.8454300254
C	-3.2557543961	2.0030938476	0.6889604609
H	-1.9441710543	2.1738412991	-1.033225049
H	-1.3429013065	2.9677942988	0.414961766
H	-3.7897947138	1.1318185191	0.2863426904
C	-4.0992644238	3.2693683823	0.4757543022
H	-3.1449145505	1.8207355085	1.7661080893
C	-4.4533098168	3.5444247195	-0.990293548
H	-3.5640056709	4.1340524191	0.8918817661
H	-5.0258574807	3.1769904852	1.0565896889
H	-5.10983726	4.4156930343	-1.0827443313
H	-4.9719282437	2.6869335159	-1.4350432315
H	-3.5617464903	3.7406828698	-1.5944312952
C	2.9744074244	0.1503712202	0.5985875842
C	2.4360277481	0.0444670495	2.0440146586
H	1.69108843	-0.7531432239	2.1281061791
H	3.2531403731	-0.1807330707	2.7387955533
H	1.968326567	0.9753147517	2.3773018243
C	3.6566518885	-1.1848781185	0.2479602215
H	4.4776645351	-1.3751874837	0.946956829

H	2.9616489862	-2.0279490934	0.3166397117
H	4.0795473093	-1.1705034925	-0.7618120155
C	4.0430548691	1.2668205026	0.5385777833
H	4.4491339286	1.3605723918	-0.4739950033
H	3.6218611813	2.2366862718	0.8195645707
H	4.8727673911	1.0476633839	1.2208377918
H	4.8727673911	1.0476633839	1.2208377918

TS exo 0247

E(RB3LYP) = -706.413961981 A.U.

First frequency = -487.1834 cm^{-1}

H	0.5559117493	-1.8196231834	-2.3923255727
C	0.7626066222	-0.8379095421	-1.9766615235
H	0.3195422773	-0.0193208112	-2.5307002618
C	1.8737981287	-0.6605378309	-1.1719561528
C	2.1405167308	0.5519749188	-0.4952739342
C	1.2967060841	1.6277828253	-0.7456454784
H	1.4029007013	2.5548468123	-0.190431746
H	0.8594359658	1.7553978869	-1.7274374292
C	-0.7819672828	0.9458439964	-0.159285997
H	-0.5221030823	1.2299671877	0.8569406887
C	-1.5944154679	1.9510775844	-0.9483561814
C	-0.8884886422	-0.4167853731	-0.4257979454
H	-1.5856186495	-0.7258991203	-1.2006834834
C	-0.5574023653	-1.4138160443	0.6620077204
H	2.4248193444	-1.5510864288	-0.8890682856
H	-1.2462340617	-1.251582844	1.5059051834
H	0.4422524012	-1.171205004	1.047375153
C	-0.6050819179	-2.8969086632	0.2745790064
H	0.1329885504	-3.0961610598	-0.5115488347
C	-1.9826849631	-3.3888365185	-0.1871979055
H	-0.2930856844	-3.4928094203	1.142995524
H	-2.2953125584	-2.8363045804	-1.0821077523
H	-2.7266081352	-3.1580630367	0.587758004
C	-2.0018299223	-4.8896575736	-0.4915516435
H	-1.7299499911	-5.4749974405	0.394361604
H	-1.2850440853	-5.139087106	-1.2824930939

H	-2.9913981348	-5.2226304726	-0.8212117125
C	-3.0842271521	1.9845303306	-0.5515099565
H	-1.5223176001	1.7111195434	-2.0184082514
H	-1.1715665046	2.9568081269	-0.8289151421
H	-3.6144827363	2.6820225838	-1.2151226625
C	-3.3318188005	2.392614642	0.9052984844
H	-3.5227768076	0.9930438063	-0.7277444641
C	-4.8205825196	2.4628918622	1.2563329847
H	-2.8608229359	3.367846347	1.0921602395
H	-2.832210905	1.6791892675	1.5724129691
H	-4.9754608276	2.7532155405	2.3006567733
H	-5.3058479207	1.4918463302	1.1045576109
H	-5.3413856125	3.1927897948	0.6258642156
C	3.1940241891	0.6529576406	0.6278026866
C	4.2388566478	1.7245839307	0.2380296937
H	4.7402296006	1.4550427585	-0.6973702433
H	3.7711824926	2.7032342599	0.0950714438
H	5.0021180918	1.8249801361	1.0185709957
C	2.5183308194	1.0651737988	1.9558852716
H	3.2671357392	1.1598265638	2.7505550435
H	2.003340313	2.0265266173	1.8735495867
H	1.7835146191	0.3173138701	2.2705759856
C	3.9364668102	-0.6746956168	0.8659165918
H	4.4548582003	-1.0166517255	-0.0357245593
H	4.6893732817	-0.5421621493	1.6497468158
H	3.2557426454	-1.4680555352	1.1919020242
H	3.2557426454	-1.4680555352	1.1919020242

TS exo 0248

E(RB3LYP) = -706.413185156 A.U.

First frequency = -492.4305 cm⁻¹

H	1.1682127153	-0.9702019811	-3.2084956126
C	1.0552424274	-0.2173734312	-2.4327180803
H	0.3394849803	0.5615423186	-2.6707398817
C	2.0993690891	0.0005200896	-1.5485361623
C	1.9786285277	0.852271576	-0.4270763909
C	0.8048393602	1.577561041	-0.2822401676

H	0.6375345693	2.1759952439	0.6066435322
H	0.2534078888	1.9112467491	-1.1514564542
C	-0.9003525407	-0.0120065791	-0.2220208977
H	-0.674039625	-0.0940096314	0.838138705
C	-2.0893433104	0.853168971	-0.5902999331
C	-0.4978654931	-1.0540736495	-1.0532065018
H	-1.1021742155	-1.2416079535	-1.9387898588
C	0.2439858663	-2.2408706727	-0.4767837202
H	2.9402432363	-0.6823212965	-1.599046184
H	1.0980001435	-1.8679200695	0.1018076896
H	0.6637037793	-2.8493143027	-1.2874598816
C	-0.6231827483	-3.1334587599	0.4320404511
H	0.0081279311	-3.9238707029	0.8621146231
C	-1.8161215388	-3.7772564961	-0.2835536854
H	-0.9906877581	-2.5369593542	1.2780650511
H	-1.4521513057	-4.3493627996	-1.1484738078
H	-2.4623636778	-2.9887327313	-0.6897631271
C	-2.636631211	-4.6907336602	0.6310913842
H	-3.0350687131	-4.1337150559	1.4869802888
H	-2.0222678105	-5.5072166064	1.0279105602
H	-3.4839062474	-5.1380466471	0.1009307578
C	-2.4255659032	1.9580820165	0.4167536465
H	-2.9738059737	0.2069425268	-0.6996569368
H	-1.9331601837	1.2962923326	-1.5859615188
H	-2.5379476805	1.5107918936	1.4147899849
C	-3.7015084761	2.7288701149	0.06131312
H	-1.590274631	2.6639310698	0.492830846
C	-4.0319859125	3.8330315161	1.0694373988
H	-4.5433441497	2.0262574129	-0.005415892
H	-3.5913258538	3.1660795548	-0.9406054032
H	-4.9463865419	4.3689555421	0.7951398749
H	-3.2201751737	4.5669654492	1.1298648204
H	-4.1762656885	3.4185909263	2.0738023364
C	3.0110533123	0.8451673723	0.721292105
C	3.5663764679	2.2759875335	0.9097008691
H	2.7698288432	2.9858561227	1.1510421957
H	4.3003969529	2.3029277258	1.7234841005
H	4.0575247454	2.6247174847	-0.0047309319

C	2.3348146357	0.3860492859	2.0337978781
H	3.0565712684	0.395436371	2.8585807904
H	1.5030168248	1.0378340986	2.3157902223
H	1.944174551	-0.6321771564	1.937358269
C	4.1992326523	-0.0944996893	0.4454740752
H	4.7277509059	0.1800244091	-0.4732249027
H	4.9165343295	-0.0353196221	1.2705748076
H	3.8810145082	-1.1385858658	0.3593992746
H	3.8810145082	-1.1385858658	0.3593992746

TS exo 0249

E(RB3LYP) = -706.413374163 A.U.

First frequency = -514.2085 cm⁻¹

H	1.0426433357	-0.5553038899	-3.3261815709
C	0.9289482948	0.0855496132	-2.4553406639
H	0.3530285666	0.9856117446	-2.644339526
C	1.9059872319	0.0567311359	-1.4698032095
C	1.7708483854	0.7499879321	-0.2457153288
C	0.6632837123	1.5681506167	-0.082148929
H	0.4623124589	2.0538116108	0.8636588668
H	0.2284052533	2.0683813654	-0.9375575927
C	-1.1934217723	0.1919061053	-0.4454671491
H	-1.0895622998	-0.098285582	0.5970972855
C	-2.2454253539	1.238724931	-0.7505431712
C	-0.810321402	-0.7336494713	-1.4179365404
H	-1.3564719208	-0.7038849706	-2.3608856749
C	-0.2927194901	-2.0915343874	-0.9977147179
H	2.6752230418	-0.7075709464	-1.5482326631
H	0.4733768438	-1.9410183777	-0.2314947774
H	0.2074423087	-2.5870233438	-1.8395177226
C	-1.3960006263	-3.0157401716	-0.4524334715
H	-1.8816827069	-2.5275256932	0.4034625802
C	-0.8894807527	-4.4033038257	-0.0288988946
H	-2.1749915706	-3.1318240557	-1.2178544743
H	-0.4075014947	-4.8903224224	-0.8879126381
H	-1.7514371923	-5.0305775176	0.2322176177
C	0.0850647442	-4.3744594499	1.1549453249

H	-0.3662463803	-3.8743371376	2.020226968
H	1.0080206983	-3.8391505206	0.9110386515
H	0.3640861048	-5.3871291472	1.4639977007
C	-2.5698859949	2.1921678469	0.4044501306
H	-3.1748113589	0.7277481589	-1.046007355
H	-1.9452637455	1.8205970883	-1.6359798041
H	-2.8259629911	1.6011987478	1.2954955142
C	-3.7208944021	3.1526741319	0.0865404323
H	-1.6807947956	2.774885883	0.6718883276
C	-4.0397923177	4.1052436964	1.2422774492
H	-4.6173737064	2.5724477231	-0.1712903215
H	-3.4677367553	3.7342381622	-0.8105877666
H	-3.1692693672	4.7205505037	1.4971108956
H	-4.3249030474	3.5496198915	2.1430226612
H	-4.8641324878	4.7809197015	0.9922016851
C	2.7451274385	0.4302110453	0.9079274858
C	4.1846214658	0.7424092583	0.4375028841
H	4.9032342585	0.5309726593	1.2377251941
H	4.4678537502	0.141699077	-0.4315843927
H	4.2818057327	1.7969853709	0.160107055
C	2.4602941157	1.2744266381	2.1636858435
H	1.4705328587	1.0606278635	2.5804549383
H	3.1987936852	1.0474765392	2.9396495428
H	2.5172729796	2.3464463229	1.9497272276
C	2.6537598939	-1.0607457147	1.3087770406
H	3.3697716938	-1.2889146185	2.1067710348
H	1.6517883874	-1.3044306908	1.6768205947
H	2.8723827894	-1.7232345332	0.4663706399
H	2.8723827894	-1.7232345332	0.4663706399

TS exo 0255

E(RB3LYP) = -706.415120342 A.U.

First frequency = -496.1586 cm⁻¹

H	-0.0978093526	-0.8145288254	-2.8379334493
C	0.2933545944	-0.0734999144	-2.1471918242
H	-0.0092058918	0.942322489	-2.3696043918
C	1.442023542	-0.3553699246	-1.4279685299

C	1.9368999181	0.500406123	-0.418609525
C	1.2869717111	1.7173729718	-0.2359699639
H	1.569354814	2.3776545859	0.5786605549
H	0.8675671697	2.2349378518	-1.0893474393
C	-0.8534160467	1.2460205697	0.2621580553
H	-0.536290787	1.1496945606	1.2989831271
C	-1.5075057698	2.564438353	-0.0900145142
C	-1.1936649007	0.0648044473	-0.3981553658
H	-1.9626367541	0.1031436131	-1.1659863126
C	-0.9754254852	-1.2562205637	0.2998165386
H	1.8304873912	-1.3659804213	-1.4956801841
H	-1.5507607675	-1.264182712	1.2390473429
H	0.0788084423	-1.3036003565	0.6011699539
C	-1.3482565624	-2.4980295765	-0.5140258327
H	-2.3938717001	-2.4094705951	-0.8389719011
C	-1.1652721558	-3.8183709099	0.2493033784
H	-0.7437603361	-2.5273091498	-1.4284905934
H	-1.5537197987	-4.6395369364	-0.3662971704
H	-1.7805595576	-3.8021725193	1.1594211584
C	0.2911680325	-4.120474208	0.6234691866
H	0.6920842699	-3.3823388394	1.3254530676
H	0.9331222482	-4.1121322042	-0.2655302251
H	0.3853507371	-5.1046642701	1.0937359565
C	-2.811897173	2.8293374018	0.6956726844
H	-1.7074582358	2.5960394759	-1.1691337985
H	-0.8219483087	3.3957273048	0.1152033061
H	-2.5753482993	2.8174926158	1.7681339795
C	-3.9631217711	1.8481950996	0.4284288047
H	-3.1527181094	3.8491658038	0.4684776764
C	-4.5003158411	1.8935455459	-1.0060555041
H	-4.7814982938	2.0764058471	1.1230527947
H	-3.6347075481	0.8291536875	0.665359878
H	-4.8315881049	2.9046634801	-1.2704751624
H	-5.353797946	1.2192036293	-1.1307871202
H	-3.7400832369	1.5971061692	-1.7359773754
C	3.0203396143	0.0507698882	0.5837364998
C	2.4644522677	0.0939556986	2.0257964282
H	3.2413240448	-0.1974901909	2.7417786191

H	2.1200863363	1.0942651595	2.3034448248
H	1.6215322551	-0.594566112	2.1425775509
C	3.5227424513	-1.3791620114	0.3118825455
H	4.3079115038	-1.6379077642	1.0298104439
H	2.7224624704	-2.1189052837	0.4161466975
H	3.9489777009	-1.4744335804	-0.692084232
C	4.2269368181	1.0126861877	0.4789910894
H	4.6474493743	0.9982926916	-0.5319250838
H	3.9354881761	2.0429960678	0.7037983567
H	5.0167456594	0.7232849994	1.1820856006
H	5.0167456594	0.7232849994	1.1820856006

TS exo 0260

E(RB3LYP) = -706.413261578 A.U.

First frequency = -501.9942 cm^{-1}

H	0.1893277197	0.1197804368	-3.1123064428
C	0.3599077387	0.6104035903	-2.1577465661
H	-0.2746930826	1.468145707	-1.9773992424
C	1.5880516099	0.4669876024	-1.53439349
C	1.837983327	0.9342088846	-0.2244062539
C	0.8233898713	1.6333144183	0.4174261155
H	0.9274555393	1.9286754546	1.4570287332
H	0.1525844302	2.2632146791	-0.1517736746
C	-0.9429958456	0.2117998164	0.5128593851
H	-0.4331092326	-0.2708431085	1.3434584338
C	-2.0228545697	1.1919324356	0.9379305839
C	-0.9754779112	-0.5004607069	-0.6854187414
H	-1.8044873124	-0.3280924446	-1.3668997488
C	-0.3300152259	-1.8663066299	-0.7571940749
H	2.2902130121	-0.2276699876	-1.9824797678
H	0.6776701226	-1.8026565175	-0.3254648831
H	-0.1954685118	-2.170306575	-1.8024253991
C	-1.1251455023	-2.9522792753	-0.0119425981
H	-1.2526250546	-2.6507321291	1.0365533471
C	-0.457712784	-4.330875538	-0.0707434441
H	-2.1385204149	-3.0174937823	-0.4326889562
H	0.5557243746	-4.2573538884	0.3475869417

H	-0.3307433613	-4.6275074264	-1.1209070133
C	-1.2457185072	-5.4101796171	0.6768956111
H	-2.2518492388	-5.524485722	0.2573977371
H	-1.358641561	-5.1520848923	1.7361360374
H	-0.7486873106	-6.3843189062	0.6219367603
C	-2.7025120982	1.9879674888	-0.1831657584
H	-1.6087270146	1.8986970358	1.6691956482
H	-2.7982793124	0.6314718514	1.4836816654
H	-1.9497624227	2.5393285178	-0.7624246498
C	-3.7481543119	2.9777727074	0.3431872478
H	-3.1865154765	1.3021035357	-0.8901696259
C	-4.4373947836	3.767260503	-0.7731084578
H	-3.2668279871	3.6733871082	1.0439282932
H	-4.5006168627	2.4306716121	0.9273426913
H	-5.1779881575	4.4672927524	-0.3731029191
H	-4.9537761891	3.0964105501	-1.4692275829
H	-3.7096316838	4.3464647734	-1.3529776559
C	3.0861259008	0.5022232549	0.5742397999
C	4.0619266936	-0.3453453655	-0.2625629294
H	3.612256659	-1.292627035	-0.5773433607
H	4.3969038523	0.189470337	-1.1572567313
H	4.9489031366	-0.5840928087	0.3333498425
C	3.8402801552	1.7637669025	1.0547361173
H	4.1605022873	2.3718802327	0.2022934219
H	3.2087558121	2.3899752548	1.6916623919
H	4.7308681581	1.4870191344	1.6309686385
C	2.6604164589	-0.3339618156	1.803260817
H	2.1357063205	-1.2439573337	1.4941345358
H	3.5394529668	-0.6312583199	2.3865736283
H	1.9966236497	0.2255923224	2.4686902149
H	1.9966236497	0.2255923224	2.4686902149

TS exo 0271

E(RB3LYP) = -706.412942282 A.U.

First frequency = -517.2340 cm^{-1}

H	1.6989116416	-0.5965571443	-3.3028814612
C	1.4541782034	0.1022458055	-2.5067277163

H	0.8550231978	0.9462176882	-2.833405045
C	2.3214817514	0.2193994433	-1.4280775951
C	2.0170119687	1.0020370943	-0.2921810989
C	0.8506406644	1.7516658854	-0.3163296805
H	0.5202590187	2.3018184101	0.5551640207
H	0.4807056187	2.146213698	-1.2532165225
C	-0.8483598711	0.2057318161	-0.7264561428
H	-0.7942986964	-0.0081717661	0.3354353378
C	-1.9401070534	1.1577207182	-1.1781064011
C	-0.3284943852	-0.7527761774	-1.6003910532
H	-0.7907940389	-0.8070653669	-2.5870876334
C	0.2000717987	-2.0710048573	-1.0719904667
H	3.1359749301	-0.4973617192	-1.3593608705
H	0.759490402	-1.8835556424	-0.1480092068
H	0.917395362	-2.4989323181	-1.7818226654
C	-0.8977816283	-3.1206870707	-0.8000250104
H	-1.4611039008	-3.3027835596	-1.726607572
C	-1.880298657	-2.7663419059	0.3224702355
H	-0.408190044	-4.0732278484	-0.5526698199
H	-2.4239139823	-1.8515871292	0.0611843421
H	-1.3147133375	-2.5325138275	1.2356105023
C	-2.8795870625	-3.8908210119	0.6093809647
H	-2.3663060339	-4.8102346293	0.9138887565
H	-3.4729837238	-4.1258213153	-0.2818879085
H	-3.5752896248	-3.6161562378	1.4091167685
C	-2.5486026798	2.0159720774	-0.0596695138
H	-2.7504061701	0.5790047348	-1.6467577144
H	-1.5566807333	1.8107397386	-1.9761403154
H	-1.7562660521	2.5790036852	0.4492332552
C	-3.3411635475	1.2072401473	0.9763963752
H	-3.2160087164	2.7645830786	-0.5065450838
C	-3.94625368	2.0840278348	2.0762348807
H	-2.6941570092	0.4474512312	1.4322693019
H	-4.1391690602	0.6535747456	0.4625413324
H	-4.6260072275	2.8333213355	1.6544539652
H	-3.1643057722	2.6215585223	2.6249626812
H	-4.5126331004	1.4891826242	2.8001281026
C	2.8671340606	0.8317882235	0.9840808826

C	2.7703440542	-0.6196792892	1.5085215046
H	3.393427431	-0.7494123139	2.4010868085
H	1.7381334224	-0.8653636379	1.7797488122
H	3.1023329084	-1.3450838155	0.7605624458
C	4.3410026581	1.1559889843	0.6487557821
H	4.9690008747	1.0457687713	1.5402948474
H	4.7396458201	0.4909458809	-0.1226038669
H	4.4393169461	2.1842615599	0.2860736864
C	2.4173412793	1.7752581248	2.1148974467
H	3.0749019116	1.6562035848	2.9823467185
H	2.4578119524	2.8240569486	1.8039134177
H	1.3967546437	1.5555997091	2.4452938094
H	1.3967546437	1.5555997091	2.4452938094

TS exo 0276

E(RB3LYP) = -706.411845703 A.U.

First frequency = -511.4884 cm⁻¹

H	1.121683419	-0.9552136232	-3.0130716629
C	1.0925299691	-0.1597976059	-2.2729881018
H	0.4376682841	0.6640161931	-2.5331960607
C	2.1832387346	0.0269242629	-1.4380843606
C	2.1670055004	0.9319467451	-0.353131712
C	1.0283357907	1.7107242515	-0.1862867796
H	0.9110823206	2.3601608707	0.6730220466
H	0.476345138	2.0390453671	-1.0577995934
C	-0.6998058177	0.2783402846	0.0396498002
H	-0.4182855465	0.1383328358	1.0813578499
C	-1.8238370222	1.2627477737	-0.2025824017
C	-0.4891412038	-0.8002440912	-0.8244113386
H	-1.161367881	-0.8876595405	-1.6747047438
C	0.1412643118	-2.0753739893	-0.3023234986
H	2.9790003756	-0.7129375186	-1.4796971424
H	1.0506461699	-1.7867250988	0.2360781665
H	0.4723583741	-2.7049359426	-1.1377249969
C	-0.7273608635	-2.9266614691	0.6537222597
H	-0.0497105865	-3.5606117752	1.241143154
C	-1.7626241077	-3.8468153392	-0.0137650398

H	-1.229780384	-2.2662453212	1.373130395
H	-2.1445949251	-4.541827721	0.7456812866
H	-1.2520799259	-4.4697681193	-0.7614575329
C	-2.9546116495	-3.1399601328	-0.6670467414
H	-2.646250321	-2.5034304423	-1.5009150187
H	-3.476078511	-2.5047403142	0.0570742556
H	-3.676800482	-3.8660794662	-1.0556630955
C	-3.1937939513	0.7245806357	0.2499950565
H	-1.876173504	1.5013423236	-1.2751644122
H	-1.6136364406	2.2069104065	0.3121175845
H	-3.3941122269	-0.2074865757	-0.2899894162
C	-4.3598519219	1.7008043274	0.0292000503
H	-3.14004426	0.4554413642	1.3146263589
C	-4.2889634229	2.9710945749	0.8846637886
H	-5.3002271081	1.1776606366	0.2449895583
H	-4.4024876364	1.9761676109	-1.0337593614
H	-3.4118117859	3.5789858105	0.6410789291
H	-4.2326798215	2.7217182575	1.950785358
H	-5.1735878881	3.5987789653	0.7355040965
C	3.2954251525	0.8688151595	0.6963846957
C	3.3421983385	-0.5227042808	1.3696889565
H	4.1593707324	-0.5701952877	2.0988860229
H	2.4059620907	-0.729606172	1.898603128
H	3.5001191728	-1.3221471372	0.6403447981
C	4.6436743061	1.1360826187	-0.011891823
H	4.848758207	0.3941349565	-0.788958397
H	4.6446249305	2.1234075968	-0.4848713335
H	5.4684352286	1.1008030269	0.7092169069
C	3.1207247934	1.9245987428	1.8034907159
H	3.9652332095	1.8777545417	2.4989385917
H	3.0814340215	2.9378051195	1.3909810943
H	2.2081144238	1.7562152234	2.3847151237
H	2.2081144238	1.7562152234	2.3847151237

TS exo 0277

E(RB3LYP) = -706.412008818 A.U.

First frequency = -509.9462 cm^{-1}

H	1.0017096377	-1.2289122024	-2.9972893441
C	1.0861358659	-0.3455208332	-2.3695502307
H	0.729191569	0.5647394975	-2.8389133572
C	2.0653504902	-0.3082486061	-1.3874898298
C	2.1505345338	0.7336921978	-0.4366639015
C	1.2644389115	1.7940519849	-0.565356823
H	1.2084957162	2.5786125412	0.1796416817
H	0.9374449707	2.1018497094	-1.5500042708
C	-0.8230828912	0.8620480204	-0.4856162314
H	-0.7060728593	0.828528437	0.5926047495
C	-1.5881361989	2.0356600662	-1.0625995767
C	-0.7725421093	-0.3540209139	-1.1723070983
H	-1.3426787669	-0.4146080057	-2.0994747961
C	-0.6094011719	-1.6557460111	-0.4179470372
H	2.623691377	-1.2225677699	-1.2018723005
H	0.2142664849	-1.5489191752	0.2979896896
H	-0.313163584	-2.4505478444	-1.1107993734
C	-1.8792374468	-2.0734066186	0.3452736923
H	-2.1610173317	-1.2588627466	1.0225326826
C	-1.7246587961	-3.370897258	1.1540686462
H	-2.7122523349	-2.1817573056	-0.3642764951
H	-2.6247825294	-3.5141509663	1.765629588
H	-0.8913558181	-3.2550191295	1.8610353422
C	-1.4984315282	-4.6231284106	0.2990559372
H	-0.5588820129	-4.5700917038	-0.260045352
H	-2.3089831921	-4.7519945121	-0.4279252848
H	-1.4603887568	-5.5248358557	0.919067229
C	-3.1296496002	1.959846088	-0.9415947769
H	-1.3401462626	2.103305181	-2.1313366702
H	-1.2463314748	2.9772158584	-0.6138680972
H	-3.5572339885	2.617152914	-1.7103528116
C	-3.7220131329	2.3835444018	0.4124420842
H	-3.4592532297	0.9419454375	-1.1882866677
C	-3.4385423971	1.4427156532	1.5882764511
H	-4.8098067173	2.4741206019	0.2940981436
H	-3.3615328161	3.3925962219	0.656592046
H	-2.3739648811	1.4038311969	1.8344413156
H	-3.7617721281	0.4215399268	1.3592153127

H	-3.9722074496	1.7687984045	2.4874696835
C	3.0526748509	0.5482062781	0.8006886346
C	3.0348484237	1.7800998786	1.7243636637
H	2.0403790743	1.9558836862	2.1476157551
H	3.724417708	1.6277536797	2.5612145701
H	3.345449937	2.6856217175	1.1934831008
C	2.5956908537	-0.6747120348	1.6298461692
H	2.6188907936	-1.5963133051	1.0415756653
H	3.248576412	-0.8164837976	2.498964711
H	1.5730169373	-0.5350802481	1.9957723124
C	4.507207752	0.3266884012	0.3259595064
H	4.5982158688	-0.5604663571	-0.3072724147
H	4.8621978862	1.1864571994	-0.2513704783
H	5.1738759315	0.1924122688	1.1855815757
H	5.1738759315	0.1924122688	1.1855815757

TS exo 0284

E(RB3LYP) = -706.414367099 A.U.

First frequency = -511.9637 cm^{-1}

H	0.5342196407	-1.4128772494	-2.8469030014
C	0.6921908278	-0.5270921644	-2.2391722994
H	0.3812818591	0.3947119599	-2.7168075429
C	1.6782940181	-0.5376542992	-1.2665577695
C	1.867458073	0.5296465465	-0.3589379007
C	1.0794664631	1.6616138791	-0.5296172055
H	1.1065917802	2.4796870289	0.1804116086
H	0.791460593	1.9628013333	-1.5286546339
C	-1.0698027142	0.974403987	-0.4130668048
H	-0.9807537026	1.0379909843	0.6684395696
C	-1.7288168912	2.1542149726	-1.0941612852
C	-1.1587886371	-0.3056182979	-0.9627086881
H	-1.7384441356	-0.4222188349	-1.8777628599
C	-1.0760407551	-1.5099744426	-0.0517576676
H	2.1667401881	-1.4867710797	-1.0580397319
H	-1.9071754364	-1.4623340839	0.6698803207
H	-0.1616925446	-1.4195275615	0.5446768792
C	-1.1208721651	-2.8722979465	-0.7503003932

H	-2.008644018	-2.9118264052	-1.3962956821
C	-1.1471246282	-4.0650860393	0.2173166536
H	-0.2536306351	-2.9719924664	-1.4137504632
H	-1.2943475209	-4.9862685563	-0.3606586474
H	-2.0194570445	-3.9781055971	0.879652366
C	0.1244703885	-4.2036795411	1.063257023
H	1.0131515482	-4.2701328709	0.4240216491
H	0.0927517901	-5.1049862246	1.6840606079
H	0.2642381211	-3.3483162207	1.7312930238
C	-3.2606212828	2.1933414434	-0.9035788286
H	-1.5155346589	2.1162656863	-2.1714643619
H	-1.2931514529	3.0925171434	-0.7319178855
H	-3.6545531428	3.0864913201	-1.4086917298
C	-3.7263333258	2.1954654242	0.5610082301
H	-3.6993165324	1.3257595582	-1.4125650652
C	-3.1851758457	3.368080238	1.3860052314
H	-3.4326029153	1.2502053996	1.0345396424
H	-4.8232878189	2.2162471332	0.5782749086
H	-3.4346034184	4.3280530788	0.9188014813
H	-2.0953031622	3.3235019105	1.4845948899
H	-3.6060066298	3.3693514514	2.3966926856
C	2.7907270845	0.3279197652	0.8602668544
C	2.8596766467	1.581099744	1.7520065281
H	3.213539756	2.4539642111	1.1942504021
H	1.8837163323	1.8243283402	2.1851602843
H	3.5534926852	1.4096991556	2.5816084391
C	2.3093776488	-0.8518755712	1.7363487943
H	1.3150442662	-0.6492981267	2.14788418
H	2.2548111984	-1.785762694	1.1705767029
H	2.9950444662	-1.0110610178	2.576657197
C	4.2175592364	0.0252145207	0.3457006523
H	4.9059857191	-0.1175611127	1.1866847343
H	4.2438381054	-0.8820326948	-0.2648781939
H	4.5923869044	0.8510491195	-0.2674514842
H	4.5923869044	0.8510491195	-0.2674514842

TS exo 0285

E(RB3LYP) = -706.413082146 A.U.

First frequency = -506.1464 cm⁻¹

H	0.2643499044	-1.5470062289	-2.3818521481
C	0.4382672062	-0.616916237	-1.848870452
H	-0.1555477236	0.2147817506	-2.2093994515
C	1.6536757143	-0.4127464569	-1.2168990055
C	1.9150728766	0.7143170047	-0.4048228436
C	0.9269746347	1.686285411	-0.3208838198
H	1.0194383088	2.5286966727	0.3542353549
H	0.2985257847	1.8834419675	-1.1797889461
C	-0.938444817	0.6384715592	0.4414144667
H	-0.5446409635	0.7541948171	1.4489779928
C	-1.9651762349	1.6661246216	0.0189708855
C	-0.9669047437	-0.6532553964	-0.0866142358
H	-1.7641719962	-0.8756472695	-0.7927644916
C	-0.4481754596	-1.8081431957	0.7447778383
H	2.3389065123	-1.2558219505	-1.1662893914
H	-1.1482945396	-1.9588247525	1.5819590129
H	0.4991970027	-1.5009799708	1.2026945314
C	-0.2503890036	-3.1572445828	0.0398088997
H	0.5678918077	-3.0809316089	-0.6856802729
C	-1.4992616991	-3.70114731	-0.663704384
H	0.0785155057	-3.8895729609	0.7897737402
H	-1.8003442759	-3.0147428602	-1.4649966129
H	-2.3358561267	-3.7249140587	0.0483724657
C	-1.2828074779	-5.0974498204	-1.2544417555
H	-1.0172012158	-5.8192286704	-0.4735654806
H	-0.4672031905	-5.0913762647	-1.9868898811
H	-2.1814256994	-5.4667150322	-1.7593595375
C	-3.3202967667	1.4702149456	0.7252994297
H	-2.1217829796	1.6018374811	-1.0681932649
H	-1.5918096653	2.677170472	0.2167875682
H	-3.6685370369	0.4483307642	0.5293148151
C	-4.406107014	2.4695517408	0.2966877304
H	-3.1709371483	1.5380107211	1.8122498307
C	-4.1087138575	3.9240888048	0.6793085097
H	-5.3589132325	2.1687314126	0.7507950254
H	-4.5514662669	2.3989050022	-0.7902380192

H	-3.9430635282	4.0185274547	1.7589538381
H	-4.9416686798	4.5821712845	0.4111511398
H	-3.2153956987	4.3043714538	0.1737320947
C	3.1733203599	0.7213666343	0.4870471382
C	3.1492943328	-0.4608241753	1.4835077423
H	4.0649881838	-0.4752402539	2.0860715887
H	2.2984186809	-0.3740010463	2.1671346
H	3.0720970448	-1.4238396238	0.9709710329
C	4.4199879793	0.5955453608	-0.4194285021
H	5.3346970699	0.6045677277	0.1845070884
H	4.411372008	-0.333682544	-0.996413117
H	4.4697497364	1.4280631391	-1.1285946436
C	3.3041447028	2.022907591	1.2991553482
H	3.3327633506	2.902388257	0.6480105444
H	2.4754960316	2.1462488327	2.0042658489
H	4.2308663721	2.0063731447	1.8822461888
H	4.2308663721	2.0063731447	1.8822461888

TS exo 0286

E(RB3LYP) = -706.413176221 A.U.

First frequency = -498.3494 cm⁻¹

H	0.3706338299	-0.0323082768	-3.087333283
C	0.5057855064	0.4966230894	-2.1477555389
H	-0.2165498551	1.2823953981	-1.9696078235
C	1.75379445	0.5033025386	-1.5487307513
C	1.976630407	1.0252515902	-0.2544339742
C	0.9033078649	1.6209635331	0.3965189382
H	0.9961850003	1.9507505468	1.4268013625
H	0.1546119344	2.1593864609	-0.1696556606
C	-0.6864877673	0.0174891104	0.5682662151
H	-0.107505515	-0.3930847008	1.392323496
C	-1.8561726489	0.8816657873	1.0081367696
C	-0.6750004753	-0.7166846724	-0.6171373571
H	-1.5292675646	-0.6336040639	-1.2822940829
C	0.10629542	-2.0120900184	-0.6844715409
H	2.5199223186	-0.1191709213	-1.9981122304
H	1.124922269	-1.8238681355	-0.3227705822

H	0.2048144202	-2.3384416272	-1.7271595186
C	-0.5157495703	-3.1514287325	0.1466593245
H	0.1455741869	-4.0283241817	0.1015631013
C	-1.921285099	-3.5578094064	-0.3105519039
H	-0.5547226347	-2.8477231263	1.2017471361
H	-1.8887681381	-3.8348759496	-1.3736142486
H	-2.5883414735	-2.6889696157	-0.2423715258
C	-2.5022657948	-4.714878543	0.5066711764
H	-3.5062790584	-4.987181266	0.1647674001
H	-2.5717570121	-4.4497585771	1.5680248718
H	-1.8705363098	-5.6075649087	0.4319571051
C	-2.6614312896	1.5588293222	-0.1076143325
H	-1.5019428949	1.653434918	1.7042860691
H	-2.5422605658	0.2531533702	1.5975424227
H	-1.9963868979	2.1670598049	-0.7353366795
C	-3.7886188845	2.4472766342	0.4309927045
H	-3.0939763469	0.7992377782	-0.7713545418
C	-4.6043990292	3.1148591717	-0.679517043
H	-3.3600505019	3.2166377873	1.0874766875
H	-4.4522897404	1.843085164	1.0644472114
H	-5.0703383169	2.3662965694	-1.3305320063
H	-3.9686181316	3.748258565	-1.3087626687
H	-5.4016103095	3.7440996672	-0.2708316774
C	3.2810603746	0.7532593639	0.5243337381
C	4.330995361	0.0068499754	-0.319108287
H	5.2511357051	-0.1170012366	0.2612544557
H	3.9874305738	-0.9918072433	-0.6076948511
H	4.5844078668	0.5589923928	-1.229965042
C	3.8960321005	2.1008207225	0.968211222
H	4.129366892	2.7252357696	0.0994974063
H	3.2099351403	2.6635180733	1.607906593
H	4.8228342635	1.9370701596	1.5303049607
C	2.9761581452	-0.1028189101	1.7752908999
H	3.894107737	-0.2889802804	2.3445378998
H	2.2665427653	0.3910530412	2.445443029
H	2.5508978973	-1.0710925743	1.491624437
H	2.5508978973	-1.0710925743	1.491624437

TS exo 0288

E(RB3LYP) = -706.413496943 A.U.

First frequency = -497.5575 cm⁻¹

H	0.9432489036	-0.5677918255	-3.4249788603
C	0.866852966	0.0605353087	-2.5412666246
H	0.2813099254	0.9614272534	-2.6875245441
C	1.8582173635	-0.0151799627	-1.5753589456
C	1.7593976156	0.6531962505	-0.334211013
C	0.6884902419	1.5146231801	-0.1419754264
H	0.5277135538	1.9818253122	0.8235648306
H	0.2687068202	2.0635369675	-0.9748820645
C	-1.2166677109	0.2093900802	-0.4624671351
H	-1.1025534715	-0.0463993825	0.5877706112
C	-2.2373317504	1.280940379	-0.7876032894
C	-0.8746160717	-0.7565396583	-1.4058733656
H	-1.4268091256	-0.7545016626	-2.34464306
C	-0.3177424607	-2.0857070808	-0.9511701318
H	2.6016694695	-0.7959081521	-1.6919851813
H	0.5087169955	-1.8856081431	-0.2605379237
H	0.1177502836	-2.6267229341	-1.8005992648
C	-1.3588523102	-2.9836065552	-0.2590192397
H	-1.7872384858	-2.4433480655	0.5959639703
C	-0.7930397612	-4.3292089089	0.221570978
H	-2.1914241802	-3.1657879755	-0.9513302378
H	-0.3716871191	-4.8725333975	-0.6354756134
H	-1.6192968558	-4.9464776623	0.596814783
C	0.2717982393	-4.2001278911	1.3179000732
H	1.1667609574	-3.6817068433	0.9589914583
H	0.5874409196	-5.1829830455	1.6828073962
H	-0.1148692539	-3.6346355145	2.1741582689
C	-2.5218009849	2.2701854842	0.347631018
H	-3.1843523092	0.7940041939	-1.0664228178
H	-1.9231868395	1.8330116943	-1.6870227174
H	-2.8000152377	1.7084722884	1.2508652387
C	-3.6333319951	3.2698330116	0.0108162453
H	-1.608991941	2.8214812099	0.6022921191
C	-3.9129410909	4.2571257612	1.1474107155

H	-4.5525638279	2.7211275868	-0.2356450613
H	-3.3575585137	3.822861128	-0.8976142584
H	-4.7093851346	4.9604990063	0.8837014375
H	-3.0181487644	4.8416798978	1.3903136908
H	-4.219918227	3.7314003733	2.0588453118
C	2.6779983609	0.3066034182	0.858183345
C	3.4327486768	1.5826231048	1.2975377364
H	4.0462951961	1.9716426592	0.4782056506
H	2.7382473963	2.3729183003	1.5974430497
H	4.0918094293	1.3709355912	2.1476381984
C	1.8340122769	-0.216716099	2.0437932139
H	1.3023332355	-1.1345911001	1.7736293094
H	2.4801192329	-0.4412389106	2.9001415099
H	1.0919127976	0.5153631254	2.374566428
C	3.7215077516	-0.7709333417	0.5105569856
H	4.3673223337	-0.4588386634	-0.3165716413
H	4.3624848972	-0.9583862871	1.3781711461
H	3.2493759237	-1.720590975	0.2374330442
H	3.2493759237	-1.720590975	0.2374330442

TS exo 0290

E(RB3LYP) = -706.414907917 A.U.

First frequency = -491.4547 cm^{-1}

H	0.6240809708	-1.0428876264	-3.0550322255
C	0.7366007015	-0.2406963974	-2.3318937355
H	0.3667308366	0.7185670767	-2.6727722803
C	1.6995240119	-0.3464362833	-1.3440504158
C	1.8211474786	0.5929079651	-0.2947357924
C	1.003161813	1.7170699604	-0.3410498185
H	0.9942113278	2.4275686387	0.4801982681
H	0.7402229433	2.1530520605	-1.2963700394
C	-1.1191088691	0.9608366977	-0.3431749702
H	-1.0431870905	0.9352712139	0.7408752535
C	-1.8159163569	2.1687127594	-0.9307578943
C	-1.1469660883	-0.2684231835	-0.9980941006
H	-1.7079591872	-0.3460274386	-1.927825979
C	-0.9431623649	-1.5342382346	-0.2007595573

H	2.2190289834	-1.2951425657	-1.2613252885
H	-1.729324392	-1.603523793	0.5677356285
H	-0.0006632415	-1.4306436707	0.3519016295
C	-0.9372771316	-2.8311547652	-1.0140818115
H	-1.871552145	-2.8956745398	-1.5882333355
C	-0.7789263274	-4.0984716384	-0.1605694613
H	-0.1259857105	-2.7931357221	-1.750789997
H	-0.8933462191	-4.9772336656	-0.8077643057
H	-1.5966445983	-4.1503575378	0.571410821
C	0.5665456627	-4.188520962	0.5702420101
H	1.4014026291	-4.1077688703	-0.1361503139
H	0.6687371335	-5.14121125	1.099956559
H	0.6824701332	-3.389050312	1.3089918301
C	-3.3501839207	2.1321922804	-0.7618339605
H	-1.5867961753	2.2337840108	-2.0033626138
H	-1.4221410712	3.0871689687	-0.4804304896
H	-3.772735334	3.051099052	-1.1919520097
C	-3.8334360545	1.9856325629	0.68966003
H	-3.7479532468	1.2973518353	-1.3525692947
C	-3.3461509586	3.0975753915	1.6248895288
H	-3.5106526851	1.0126242782	1.0808396008
H	-4.9305293387	1.9654795332	0.6917135183
H	-3.7798456212	2.9930568294	2.6246594039
H	-3.6241449801	4.0864184949	1.241531502
H	-2.2567586963	3.0823831446	1.7369557802
C	2.670435172	0.3153245733	0.963440414
C	3.3972627893	-1.0407312504	0.9011838009
H	4.0059110092	-1.1755973706	1.8013034375
H	2.6937992804	-1.8779283171	0.8491359938
H	4.0672802005	-1.101631953	0.0374408852
C	3.7368013693	1.4269397982	1.1016773172
H	4.3573960404	1.2616626549	1.9901811967
H	4.3930316232	1.4455456977	0.2253254136
H	3.2738275627	2.414099741	1.1919971733
C	1.7734408522	0.3170073458	2.2228589794
H	1.0195458674	-0.4748103396	2.1691966481
H	2.3783672201	0.1480511425	3.1209622691
H	1.2500342305	1.2685275047	2.3533550105

H 1.2500342305 1.2685275047 2.3533550105

TS exo 0301

E(RB3LYP) = -706.413325926 A.U.

First frequency = -484.8948 cm⁻¹

H	1.5206088479	-0.6829047925	-3.3130873797
C	1.2943191054	0.0343456815	-2.5285671853
H	0.7262644694	0.8947969384	-2.8625212617
C	2.1060777142	0.0873292163	-1.4078608388
C	1.793286544	0.8833142538	-0.2820620592
C	0.6902303358	1.7196005473	-0.3630562637
H	0.3654073389	2.2872428885	0.5020490606
H	0.3939954956	2.1476426117	-1.3117162193
C	-1.1003626476	0.2923257636	-0.7794110123
H	-1.0925464171	0.0901934932	0.2871849373
C	-2.1477576402	1.2696024432	-1.2770317996
C	-0.6220940368	-0.7153198319	-1.6133307625
H	-1.034942221	-0.7684939633	-2.6201484553
C	-0.1375670381	-2.0187569473	-1.0198657994
H	2.8672666248	-0.6790984428	-1.3123057953
H	0.5602121216	-1.7938573299	-0.2025086948
H	0.4360577011	-2.586373351	-1.7628246783
C	-1.2761116019	-2.8991402293	-0.4766173229
H	-1.8443775146	-2.3318225756	0.2728214891
C	-0.7771011625	-4.2093116989	0.1427774904
H	-1.9844987759	-3.123104378	-1.2866769678
H	-0.0664462712	-3.9778485314	0.9483137128
H	-0.2084327941	-4.7725080438	-0.6097918971
C	-1.909581492	-5.0820824516	0.6910604277
H	-2.6166537599	-5.3528917221	-0.1014364549
H	-2.4733707772	-4.5527356701	1.467780096
H	-1.5282752115	-6.0102059752	1.1294376337
C	-2.4310891214	2.504856158	-0.4056741401
H	-3.0939015743	0.7167995238	-1.389036755
H	-1.8800201001	1.5961947267	-2.2919190338
H	-1.5729696911	3.1863666932	-0.4169316228
C	-2.7984744821	2.1855150625	1.0485343047

H	-3.2600017193	3.0610906295	-0.8640573514
C	-3.1853788091	3.4342735733	1.8461662907
H	-1.9530632424	1.691285413	1.5432399318
H	-3.6261978697	1.4630747686	1.0642232043
H	-2.3627518067	4.15862433	1.8646231888
H	-3.4363560876	3.1888062384	2.8831809751
H	-4.0531861032	3.9342352397	1.4010593988
C	2.5022186832	0.6967794821	1.0767446682
C	1.4799105157	0.2376357896	2.1424999246
H	1.970285152	0.116367392	3.1151613695
H	0.6687220246	0.960441966	2.2698554556
H	1.0322597844	-0.7228793978	1.8670784622
C	3.6301773662	-0.3496010242	1.0189543358
H	4.1226523336	-0.4168853534	1.9945445019
H	3.2487891572	-1.3458850864	0.7724757807
H	4.3928787253	-0.0818687402	0.2804989323
C	3.1208261354	2.0446453713	1.5141098348
H	3.8548174225	2.3908132947	0.7789822716
H	2.357419508	2.82182551	1.6134879871
H	3.6271253423	1.9433495234	2.4811554909
H	3.6271253423	1.9433495234	2.4811554909

TS exo 0309

E(RB3LYP) = -706.412957971 A.U.

First frequency = -500.9155 cm^{-1}

H	1.6701635059	-0.6604658445	-3.3734749244
C	1.4470142468	0.0415904803	-2.5740985608
H	0.8398832083	0.885333342	-2.8839160543
C	2.3162082331	0.1305749975	-1.4964852366
C	2.0292994965	0.9132833766	-0.356323798
C	0.8878662164	1.7015971938	-0.378284034
H	0.5813257572	2.2485919123	0.5068510453
H	0.5281179475	2.1250568222	-1.3063884745
C	-0.8585311643	0.1995603214	-0.767781646
H	-0.805160246	0.0253219118	0.3010067361
C	-1.9201763547	1.1679031466	-1.2540970173
C	-0.361890092	-0.7976824206	-1.6053006975

H	-0.8165643996	-0.882390249	-2.5926627837
C	0.1881106119	-2.0862293769	-1.0322213481
H	3.1133042351	-0.6026163521	-1.4425909695
H	0.7854336413	-1.8494131659	-0.1424882133
H	0.8779198586	-2.5481851993	-1.7476803263
C	-0.8919588998	-3.1237702518	-0.6595623305
H	-1.4920223875	-3.3563562783	-1.5509613459
C	-1.8290962029	-2.7158984514	0.483391546
H	-0.3862807713	-4.0599777663	-0.3837136166
H	-2.3947336204	-1.8227990026	0.195425075
H	-1.2276455988	-2.4257925719	1.3566282417
C	-2.8016607455	-3.832017689	0.8756973007
H	-3.4659250423	-3.5192269812	1.6880479277
H	-2.2649790745	-4.7278215074	1.2088662487
H	-3.4296162508	-4.1226276969	0.0254513336
C	-2.4948407537	2.0906756626	-0.1696813765
H	-2.7507590946	0.5977336032	-1.6968020708
H	-1.5180939253	1.7752471673	-2.0784921752
H	-1.6831678348	2.6558108297	0.305273235
C	-3.2961502539	1.3506067052	0.9100088163
H	-3.1477633246	2.8352960079	-0.6438139193
C	-3.8683983295	2.2923270144	1.9731583244
H	-2.6629388466	0.597408773	1.3953075664
H	-4.1125614902	0.7934739221	0.4299468736
H	-4.5342986036	3.0376363727	1.5231827529
H	-3.067956959	2.8354595554	2.4887260123
H	-4.4411966301	1.7459657781	2.7294715522
C	2.8164878294	0.7582703428	0.9629287271
C	1.8737826821	0.251650002	2.0791875649
H	2.4192436309	0.1538093387	3.0247887931
H	1.0367174528	0.934657099	2.2499023273
H	1.4586213554	-0.7291789759	1.8252921846
C	3.9869207304	-0.2348942482	0.8428015042
H	4.5324312309	-0.2799568595	1.791079788
H	3.6395538668	-1.2475487664	0.6135884957
H	4.6966717381	0.0683638448	0.0662466149
C	3.3949473537	2.1326753473	1.3715636781
H	3.9549146797	2.0538636946	2.3107055356

H	4.0733400449	2.5123321393	0.6004190208
H	2.6033773988	2.8743704242	1.5127267022
H	2.6033773988	2.8743704242	1.5127267022

TS exo 0316

E(RB3LYP) = -706.413894814 A.U.

First frequency = -505.0106 cm⁻¹

H	0.5938713885	-1.4901935771	-2.5079793428
C	0.7569095483	-0.5749713255	-1.9468541442
H	0.1967973743	0.2755935149	-2.3171104358
C	1.9394933123	-0.4084522497	-1.2463851868
C	2.1777828507	0.6955102565	-0.3956107612
C	1.2033950423	1.683391548	-0.3394509025
H	1.2769127466	2.5097010138	0.3575276291
H	0.6225080781	1.9107346765	-1.2240601132
C	-0.7104256592	0.6560973067	0.3098693458
H	-0.3625323713	0.7350628758	1.3377290573
C	-1.7006730322	1.7120107695	-0.1286281016
C	-0.7409152217	-0.6196049027	-0.2546168571
H	-1.5049641652	-0.8041188858	-1.0068237461
C	-0.282225256	-1.808099535	0.5623305602
H	2.6061188671	-1.2652156677	-1.1793420713
H	-0.9838841981	-1.933425893	1.4002549643
H	0.6801580738	-1.5577553661	1.0235002697
C	-0.1481741757	-3.1513224578	-0.1724924757
H	0.7180291261	-3.114553534	-0.8424442166
C	-1.3839697377	-3.584551837	-0.9777027934
H	0.0756872712	-3.9249773379	0.574403383
H	-1.1844247357	-4.5689161485	-1.4197827711
H	-1.529274009	-2.9021757712	-1.8250167051
C	-2.6736004475	-3.6505490315	-0.1521940806
H	-2.9622226908	-2.6622137802	0.2206995551
H	-2.5524539467	-4.3086718642	0.7161589328
H	-3.5074876882	-4.0347285751	-0.7485985246
C	-3.0900664208	1.5219203274	0.5056429728
H	-1.8034493823	1.6843842274	-1.2233925957
H	-1.3311526471	2.7153462148	0.1193255056

H	-3.4726720153	0.5278996472	0.2370191184
C	-4.1007140125	2.594546321	0.0849361213
H	-2.9903019892	1.5219969808	1.6002007963
C	-5.4812983712	2.3946297524	0.7167298191
H	-4.1925633972	2.5939715127	-1.0099178307
H	-3.7108616826	3.5852378205	0.3559195881
H	-5.9058553704	1.4240712931	0.4356269516
H	-6.1857098354	3.1711366205	0.4010105313
H	-5.4212600181	2.4228579153	1.8107389939
C	3.3891557142	0.6605496529	0.5584255583
C	4.6779691277	0.5400108526	-0.2878541457
H	4.6851041481	-0.373297588	-0.8897651072
H	4.774785843	1.3901795514	-0.9707323423
H	5.5613088568	0.5190256926	0.3608247595
C	3.4960418104	1.9382621836	1.4108110491
H	2.6335134398	2.0558208144	2.0751002097
H	4.3908299166	1.8920501496	2.0403220536
H	3.5711334278	2.8339538479	0.7860247482
C	3.2994260228	-0.5465973109	1.5206200807
H	3.2395636509	-1.4951121623	0.9795158038
H	4.1817397579	-0.5877381075	2.169938227
H	2.4144241867	-0.4672703721	2.1604206525
H	2.4144241867	-0.4672703721	2.1604206525

TS exo 0328

E(RB3LYP) = -706.412990813 A.U.

First frequency = -524.0953 cm⁻¹

H	0.3479978727	0.1395268077	-3.1933018553
C	0.4666524018	0.5712268212	-2.2028201506
H	-0.1817907658	1.4168711293	-2.0095781563
C	1.6822462276	0.4350049371	-1.5488234358
C	1.8718031919	0.8292958052	-0.2061662495
C	0.8044691504	1.4388377903	0.4406541658
H	0.8472272093	1.6758472652	1.4969627588
H	0.128750662	2.0708963379	-0.1208305789
C	-0.8937960491	-0.0512240848	0.347191953
H	-0.3934546537	-0.5990621992	1.1404454702

C	-2.0193894332	0.8453345841	0.836835522
C	-0.8816307758	-0.644860629	-0.9202448289
H	-1.7058625367	-0.4104291297	-1.5911992995
C	-0.2723806887	-2.0178294311	-1.1222957994
H	2.4265944791	-0.2127373016	-2.0055391134
H	0.6406726031	-2.0977521125	-0.5230124378
H	0.0412570098	-2.1396291593	-2.1652554295
C	-1.2353382177	-3.1773788594	-0.7811074871
H	-2.1352437211	-3.074993364	-1.4028282924
C	-1.6598694308	-3.2944949687	0.6908199526
H	-0.759967533	-4.1203316533	-1.0866490999
H	-2.4088477116	-4.0926723675	0.7724492412
H	-2.1634920653	-2.3713746485	1.0012622046
C	-0.5046907588	-3.5983318028	1.6509506436
H	0.0210039527	-4.5141261673	1.3562489953
H	-0.8656736794	-3.7350707242	2.6755932877
H	0.2339682163	-2.7905946763	1.6690656183
C	-2.7041157744	1.7218764066	-0.2192720258
H	-1.6490873936	1.4914975771	1.6435288237
H	-2.7863956713	0.2083132468	1.3057271359
H	-1.9584869624	2.3424149302	-0.7342805552
C	-3.7840687256	2.632377131	0.3763299847
H	-3.1592393309	1.090330783	-0.9929275145
C	-4.4821739637	3.4974092486	-0.6766762763
H	-3.3315517537	3.276724723	1.1421932808
H	-4.5275024548	2.0154089592	0.8992487717
H	-4.9711617914	2.8762053008	-1.4358015955
H	-3.7642857809	4.1446087342	-1.193533373
H	-5.2469141682	4.1394547746	-0.227819597
C	3.1367439522	0.3590134186	0.540597101
C	3.1977619486	0.8993620812	1.9812137489
H	2.3773084385	0.5137212549	2.5952518277
H	4.1345814378	0.5893442387	2.4558960605
H	3.1555411656	1.9930436168	2.0022610077
C	3.1811488502	-1.1854591189	0.6082429835
H	4.0897748731	-1.5236755554	1.1198437256
H	2.3195891378	-1.5739018122	1.1614662636
H	3.1703678503	-1.6363394124	-0.3879450483

C	4.3832766889	0.8726342337	-0.215732872
H	5.2988459513	0.5527677611	0.294937383
H	4.4242993005	0.4923169365	-1.2403488404
H	4.3835975115	1.9662892431	-0.2656363238
H	4.3835975115	1.9662892431	-0.2656363238

TS exo 0331

E(RB3LYP) = -706.412707286 A.U.

First frequency = -508.2157 cm⁻¹

H	1.1144600878	-1.1518154348	-2.9472158962
C	0.9815334352	-0.3474447897	-2.2280309123
H	0.2644264448	0.405654192	-2.5376161525
C	2.0294200007	-0.0276169043	-1.3767766808
C	1.8955703659	0.9056268876	-0.3236703849
C	0.6951858043	1.5899708826	-0.2104177946
H	0.5065835614	2.251078506	0.625032815
H	0.1155511237	1.818467164	-1.0952135013
C	-0.950499439	-0.0622114879	-0.0378643652
H	-0.70329606	-0.1083179716	1.0199402929
C	-2.1760471892	0.7501745135	-0.4059876145
C	-0.5333170864	-1.1189792922	-0.8487342407
H	-1.1593518878	-1.3406483174	-1.7124041782
C	0.1943374002	-2.2998447389	-0.2411378529
H	2.8941808701	-0.6865009013	-1.3760050819
H	1.0216929106	-1.9252739715	0.3708099663
H	0.6516153567	-2.9051211014	-1.031844274
C	-0.7077907379	-3.1884744602	0.6404116651
H	-0.1065413419	-4.0224024986	1.029397523
C	-1.950675804	-3.7504820327	-0.0674326821
H	-1.0323506312	-2.6051438389	1.5116433174
H	-2.6025631551	-2.9191571666	-0.3651287886
H	-2.5263458017	-4.3450936944	0.6532280747
C	-1.6329967434	-4.6126597127	-1.29386957
H	-1.148089157	-4.0286529553	-2.0832854813
H	-2.5427787812	-5.0484664582	-1.7194776065
H	-0.9582518828	-5.4363899839	-1.0326213993
C	-2.5228012203	1.8859886625	0.5623695361

H	-3.0417021083	0.0719803168	-0.4624941394
H	-2.0624823724	1.1541580801	-1.4239427686
H	-2.5861386222	1.4802494031	1.5822398753
C	-3.8387010204	2.590993828	0.21588923
H	-1.714275674	2.6258318228	0.5795549651
C	-4.1797055499	3.7273591626	1.1839432226
H	-4.6541861184	1.8549565022	0.209182703
H	-3.7777858101	2.9853656852	-0.8077866598
H	-4.2754397904	3.3546481464	2.2102235467
H	-5.1226841229	4.2152660979	0.916848426
H	-3.3956965796	4.4933040454	1.1839312341
C	2.9994993861	0.9835679441	0.7518040078
C	3.1553639929	-0.3746840905	1.4741200411
H	3.9559488743	-0.3236562814	2.2212208187
H	2.2291631093	-0.6473651012	1.9907360671
H	3.4013511408	-1.180630912	0.7770781493
C	4.3348140359	1.3506609406	0.0640998014
H	5.1405732175	1.417220867	0.8042032287
H	4.6277793003	0.6049721683	-0.6805064556
H	4.2566156509	2.3170348453	-0.4443765279
C	2.7023054468	2.0545504357	1.8174254912
H	1.7935605422	1.8234595537	2.3829163496
H	3.52940525	2.1062860703	2.5331347674
H	2.5837405573	3.0463640915	1.3696068978
H	2.5837405573	3.0463640915	1.3696068978

TS exo 0333

E(RB3LYP) = -706.413228901 A.U.

First frequency = -500.9937 cm^{-1}

H	1.2987755276	-0.1253456178	-3.4606027836
C	1.1159817588	0.3756502401	-2.5133249082
H	0.4165336968	1.2021890256	-2.5785225007
C	2.0937723221	0.3305101035	-1.5305146605
C	1.8814733941	0.8360076084	-0.2289694637
C	0.6862677813	1.4915980262	0.0291603442
H	0.4428223835	1.8103801336	1.0369686546
H	0.1882366292	2.0571577311	-0.7472079836

C	-0.9909883121	-0.0506617368	-0.5217737503
H	-0.8433649386	-0.4226799907	0.4871286481
C	-2.159545185	0.8919267016	-0.7279290542
C	-0.5002113185	-0.8137373174	-1.5800449065
H	-1.0402583116	-0.7440698371	-2.5247816007
C	0.1987263197	-2.1328159591	-1.3318538178
H	2.9463250934	-0.315041388	-1.7102421744
H	0.8357759779	-2.0361076652	-0.4454139205
H	0.8754043943	-2.3589036791	-2.163618259
C	-0.7673312851	-3.3272602179	-1.1662719841
H	-1.3782096349	-3.4070262502	-2.0757808576
C	-1.6989482231	-3.2833046327	0.0546655355
H	-0.1690285657	-4.2482210914	-1.1198818661
H	-2.3837185441	-4.1391103652	-0.0031479661
H	-2.3266633712	-2.3857658927	0.0040126839
C	-0.9673776213	-3.3222400363	1.4007406708
H	-0.3181946622	-4.2030630959	1.4704189384
H	-1.6752085158	-3.3627689481	2.2351771155
H	-0.3375464475	-2.4397305506	1.5494368313
C	-2.615445672	1.6366874231	0.5311431572
H	-3.0141238765	0.3173084247	-1.1168137635
H	-1.919228087	1.6181702929	-1.520079718
H	-2.8208334912	0.9039208301	1.3246809233
C	-3.8612175917	2.4993618048	0.3036640316
H	-1.803397394	2.2705528715	0.9063784994
C	-4.3123075618	3.2408283042	1.5652161781
H	-4.6795545738	1.8653234217	-0.0639619614
H	-3.6565342066	3.2243032001	-0.4961371598
H	-4.5518072376	2.5372472641	2.3707848355
H	-5.2027583008	3.8497421998	1.3783658092
H	-3.5236578933	3.9068402561	1.9337410753
C	2.8349679488	0.508675099	0.9408566449
C	4.0781642857	-0.2799087101	0.4895167892
H	4.6489771752	0.2651756925	-0.2693196944
H	4.7398361557	-0.4484982888	1.3454522316
H	3.8125912707	-1.2601975515	0.0807962919
C	3.316022936	1.8289462664	1.5862629363
H	3.996564255	1.6260868511	2.4213517881

H	3.8476005324	2.4464860018	0.8547871408
H	2.4776461595	2.4166953738	1.9711110552
C	2.094238234	-0.3358683053	2.0028848769
H	1.7765142095	-1.2961466068	1.5843679376
H	2.7514225044	-0.5412132197	2.8556907331
H	1.2051627447	0.1741893963	2.3847596854
H	1.2051627447	0.1741893963	2.3847596854

TS exo 0335

E(RB3LYP) = -706.413248046 A.U.

First frequency = -503.0586 cm^{-1}

H	0.0870922088	0.1372222591	-3.1187193166
C	0.2656955085	0.5918964409	-2.1479294227
H	-0.3337025091	1.4705988705	-1.9499646178
C	1.4767747497	0.3735569662	-1.5126966486
C	1.7269344587	0.7861407883	-0.1847049804
C	0.7390506857	1.5206833318	0.4607778508
H	0.8411849136	1.7816709304	1.5097630545
H	0.1172694328	2.2049981939	-0.101583128
C	-1.0944463636	0.1984515134	0.4943841785
H	-0.6276052144	-0.3163238189	1.3308145067
C	-2.1399567458	1.2201583993	0.9068947194
C	-1.1317924968	-0.5003564725	-0.7121299964
H	-1.9414601408	-0.2951045283	-1.4072857124
C	-0.5129609242	-1.8779929462	-0.7846122069
H	2.1518912712	-0.3403022897	-1.9719256888
H	0.4972580397	-1.8170771762	-0.3643068401
H	-0.3912593129	-2.1890617741	-1.8296535357
C	-1.3182015075	-2.9507963714	-0.0289980999
H	-1.4394051273	-2.6386661575	1.0172122811
C	-0.6798173417	-4.3481493898	-0.0712877642
H	-2.3309374399	-3.0003167829	-0.4504421805
H	-0.5585479639	-4.6602056546	-1.1177996247
H	-1.3729750284	-5.0679666235	0.3825362042
C	0.6720551318	-4.4356344273	0.6479402318
H	1.0518295088	-5.4625403723	0.6565004887
H	0.5830265101	-4.1041218488	1.6894043658

H	1.4314640431	-3.8101264485	0.1677328966
C	-2.7524102214	2.063570253	-0.2182786411
H	-1.7132973029	1.8960105673	1.6599264606
H	-2.9541689313	0.6877216203	1.423367908
H	-1.9607628365	2.595304036	-0.7628649152
C	-3.7740599992	3.0845171986	0.2955685052
H	-3.2407352532	1.4111802027	-0.9533975781
C	-4.3952236971	3.9226791947	-0.8252025479
H	-3.2880682066	3.7463928441	1.0251878712
H	-4.5660362498	2.5571298999	0.8445652737
H	-3.6268203533	4.4831701494	-1.3699690605
H	-5.1198979396	4.6441374484	-0.4342115627
H	-4.9152288461	3.2868056161	-1.5508301652
C	2.9341882478	0.2617387579	0.6219507151
C	3.8650253002	-0.6333277073	-0.2166328076
H	4.2505887514	-0.1061694069	-1.0953352872
H	4.7237132407	-0.9427083349	0.3880998337
H	3.3576923839	-1.5420939113	-0.5571018923
C	3.7595371578	1.4652554571	1.1331551458
H	4.6229092106	1.1241566982	1.7163038894
H	4.1290020716	2.0656421483	0.2952536529
H	3.1588808612	2.1194110224	1.7719448729
C	2.4419564824	-0.5668451496	1.8315497986
H	3.2942536015	-0.9237655051	2.4210055588
H	1.8035408415	0.020231558	2.4980355232
H	1.8701660076	-1.4406036844	1.5026482919
H	1.8701660076	-1.4406036844	1.5026482919

TS exo 0354

E(RB3LYP) = -706.413025202 A.U.

First frequency = -500.8796 cm⁻¹

H	1.5856857092	-1.1486289315	-3.0198731168
C	1.3313908645	-0.3261763843	-2.3563601712
H	0.6895074102	0.4229766397	-2.806261111
C	2.1955685945	-0.0012350599	-1.3225866292
C	1.8704465081	0.9533808678	-0.3314778114
C	0.6782636058	1.6475640264	-0.4663469992

H	0.3408275717	2.3330293427	0.2996256004
H	0.2817361528	1.855550181	-1.451692084
C	-0.964407663	0.0102768141	-0.5173034273
H	-0.8683583632	-0.0552796568	0.5624003986
C	-2.1464582395	0.8040134084	-1.04150649
C	-0.4506274056	-1.0540919393	-1.2606224374
H	-0.9259458587	-1.251480477	-2.2204964268
C	0.1413591884	-2.2555399383	-0.5514823173
H	3.0348308455	-0.6681427836	-1.1413651454
H	0.8863480698	-1.9027051553	0.169924285
H	0.6800400496	-2.8875482085	-1.2686619379
C	-0.9044040328	-3.1101152674	0.1909858636
H	-0.3873315822	-3.9150760617	0.7323043447
C	-1.9715307636	-3.7247907679	-0.7218520345
H	-1.3973591006	-2.4919956048	0.9539137313
H	-1.4785965505	-4.3185211076	-1.5044017377
H	-2.5097350503	-2.9222353461	-1.2420789295
C	-2.9712366268	-4.600944039	0.03798241
H	-3.72520886	-5.0280044118	-0.6315025128
H	-3.4967637643	-4.0212433791	0.8056989566
H	-2.464421932	-5.4312720458	0.543194132
C	-2.4878656158	2.1255424906	-0.3328955289
H	-3.0344403887	0.1547569736	-0.9797293194
H	-2.001439584	0.9958044407	-2.1141073636
H	-1.7173298991	2.8782111546	-0.5343617786
C	-2.6842493235	2.0014525425	1.1827535693
H	-3.4123346066	2.5192581798	-0.7767563543
C	-3.1336901597	3.3156443129	1.8278553399
H	-1.7474265817	1.6738183269	1.6503859168
H	-3.4216667803	1.2137894891	1.390573159
H	-3.2614614137	3.2108415519	2.9101308862
H	-4.088061235	3.6551119048	1.4093824387
H	-2.3978693678	4.1094618474	1.6542863948
C	2.7366658356	1.0373945102	0.9421429477
C	4.1887633579	1.3762767578	0.5340099711
H	4.6131788315	0.6160108106	-0.1279739395
H	4.2305030676	2.3362870766	0.0094337183
H	4.8300283004	1.4421012737	1.4205014871

C	2.2458555119	2.1292846653	1.910835611
H	2.9123105715	2.1840236141	2.7778850024
H	2.2335027545	3.1147793997	1.4344837861
H	1.238551828	1.9176910917	2.2849115612
C	2.7214757107	-0.3108306762	1.6995483626
H	1.7042621011	-0.5676528967	2.0134389156
H	3.0987704435	-1.129421689	1.0802744832
H	3.3482310661	-0.2553586856	2.5972093125
H	3.3482310661	-0.2553586856	2.5972093125

TS exo 0360

E(RB3LYP) = -706.411752594 A.U.

First frequency = -523.1432 cm^{-1}

H	0.6988570362	-0.0007667777	-3.2428002759
C	0.7587839841	0.5186249053	-2.2898914073
H	0.1031046593	1.3770535045	-2.2126751176
C	1.9299276797	0.4423275977	-1.5514211675
C	2.0371734319	0.956016888	-0.2402367683
C	0.933096299	1.6167047613	0.2827572802
H	0.9123346036	1.9482746439	1.3139742188
H	0.2936303491	2.1936044185	-0.372976764
C	-0.7531713925	0.1169181006	0.2271200997
H	-0.2979631745	-0.3687631132	1.086242438
C	-1.9040828659	1.0433900895	0.5849689997
C	-0.6767320094	-0.5790371102	-0.9847009083
H	-1.4587739596	-0.3975006989	-1.7192086847
C	-0.0680230832	-1.9662978943	-1.0353066928
H	2.6983211534	-0.2431771111	-1.9005681984
H	0.8025304735	-1.9988023008	-0.3691134189
H	0.3098291952	-2.1756969946	-2.0424734052
C	-1.0498186962	-3.0920974886	-0.6470452761
H	-1.9219190831	-3.0559824951	-1.3157944284
C	-1.5327315271	-3.0667820855	0.8075031227
H	-0.5609277517	-4.0574533078	-0.8406358946
H	-2.0760591649	-2.1340549649	0.9974340499
H	-0.6609781985	-3.0524682455	1.4766516991
C	-2.4282524987	-4.2602343055	1.1528797015

H	-2.7668651678	-4.2222770328	2.1935369707
H	-1.8979210855	-5.2086176189	1.0085720291
H	-3.3184657987	-4.2813797772	0.513522919
C	-2.5434966488	1.808786453	-0.582151524
H	-1.5736365552	1.768517853	1.3407804014
H	-2.6777543924	0.4389185027	1.0811561855
H	-1.7615218692	2.3272773365	-1.1510676369
C	-3.5968792458	2.8380745692	-0.1433911068
H	-3.0084419572	1.1003656496	-1.2800714906
C	-4.8269180728	2.225237355	0.5362002509
H	-3.9211249007	3.4058094905	-1.0247039494
H	-3.1291378394	3.5662327996	0.5333453279
H	-5.575528256	2.9912601388	0.7628688637
H	-4.5678477838	1.7309642337	1.4777804653
H	-5.2999073903	1.4772985369	-0.1110477659
C	3.250055652	0.5548289482	0.6236852445
C	4.5457215841	0.9897907817	-0.0984462708
H	4.5602961801	2.0739462913	-0.2500315567
H	5.4248339642	0.7152815858	0.4958362497
H	4.6461675411	0.5149086213	-1.0785097922
C	3.2280449491	1.2288122929	2.0080672472
H	4.1325420231	0.9639934596	2.5656075493
H	3.1919933983	2.3196299565	1.9231317665
H	2.3696688735	0.9039761621	2.6051542118
C	3.2743225438	-0.9767672693	0.8383720411
H	4.143221858	-1.2687150241	1.4397300261
H	2.3729315114	-1.3085054527	1.3645415266
H	3.3266248265	-1.5182382381	-0.1103399473
H	3.3266248265	-1.5182382381	-0.1103399473

TS exo 0363

E(RB3LYP) = -706.412224654 A.U.

First frequency = -520.9942 cm⁻¹

H	0.3344903414	-0.34371832	-3.1423847506
C	0.4896647601	0.2669817624	-2.2567570826
H	-0.0399852967	1.2111833736	-2.2719081692
C	1.6560220746	0.1089057063	-1.5240720617

C	1.867178253	0.7421440719	-0.2787619175
C	0.8840801326	1.6120278438	0.175104429
H	0.9371856618	2.0566309349	1.1616096167
H	0.3186304173	2.1986224458	-0.5374464369
C	-1.0148897178	0.3915744679	0.3050199585
H	-0.6220332479	-0.0432898977	1.2215533598
C	-2.0110427995	1.5152949851	0.5369178219
C	-1.051631116	-0.4540193408	-0.8079112266
H	-1.8177684292	-0.2746023401	-1.5584489896
C	-0.5998108361	-1.8908196349	-0.6584289377
H	2.3133694629	-0.7118238148	-1.8010267575
H	0.3664068487	-1.8941679142	-0.1445740952
H	-0.4264958694	-2.3434615977	-1.6428851473
C	-1.6030557802	-2.758067316	0.1233738959
H	-1.7680063884	-2.3110489167	1.1133570679
C	-1.1610149083	-4.2201830374	0.2917899356
H	-2.5742483804	-2.7284979591	-0.3885386466
H	-0.9925518244	-4.6639992866	-0.6991927032
H	-1.9832723579	-4.7893322598	0.744136227
C	0.0980171037	-4.39330471	1.1502433234
H	0.3356384238	-5.4519721892	1.2974116912
H	-0.0392392734	-3.9416460604	2.1399981488
H	0.972757987	-3.920663734	0.6926155739
C	-2.5451770614	2.2142068528	-0.7213984746
H	-1.5660413457	2.2730499188	1.1960252844
H	-2.857945373	1.0992252236	1.1017993363
H	-1.7022080779	2.5420481199	-1.3424816543
C	-3.4369396704	3.4295261619	-0.4222268993
H	-3.1123445129	1.4989003927	-1.3311094273
C	-4.7382876266	3.0867428816	0.3121624526
H	-3.6815197998	3.9268876477	-1.3693239543
H	-2.8651247344	4.1596461933	0.1668002138
H	-5.3667011323	3.9744663584	0.437265067
H	-4.547545909	2.676690311	1.3089008785
H	-5.3186410691	2.3428232873	-0.2462309188
C	3.0416802678	0.2785862115	0.6077396996
C	3.1291226455	1.075049048	1.9226554576
H	4.0030929881	0.7504495081	2.4969831599

H	3.2293992326	2.1490960471	1.7364052307
H	2.2470948763	0.9179202139	2.5522059972
C	2.8971579258	-1.218865871	0.9681128089
H	3.7422108247	-1.5505502173	1.5825262223
H	1.9779675262	-1.3961843137	1.5360860676
H	2.8668412926	-1.8503596972	0.0755874468
C	4.3618896454	0.4896610844	-0.1685721175
H	5.217542785	0.1694389673	0.4370587857
H	4.381439114	-0.0819299599	-1.100898256
H	4.4982216054	1.5459239867	-0.4221053611
H	4.4982216054	1.5459239867	-0.4221053611

TS exo 0366

E(RB3LYP) = -706.413012382 A.U.

First frequency = -489.3917 cm^{-1}

H	1.1934506294	-1.3159251172	-2.8749273663
C	1.1988247698	-0.4087605753	-2.2763654893
H	0.6756276545	0.4255543526	-2.7293536858
C	2.2140357886	-0.2160605158	-1.3530386734
C	2.2112126282	0.8574949157	-0.4340062756
C	1.1987143332	1.8010439447	-0.5463442262
H	1.0917627491	2.5914411582	0.1903021762
H	0.7900440498	2.0478904028	-1.5173158864
C	-0.7580929897	0.6281255913	-0.3092072885
H	-0.5786525769	0.6959306189	0.758539961
C	-1.6867448729	1.656601278	-0.9216412189
C	-0.5777377587	-0.6165438948	-0.9107160304
H	-1.1714690074	-0.8293160769	-1.7982309131
C	-0.1404525956	-1.8077907472	-0.0864401026
H	2.8944442124	-1.0441704976	-1.1876248786
H	0.7374951505	-1.5163984056	0.5030852174
H	0.1948295487	-2.6158281981	-0.7458610101
C	-1.223356199	-2.3356707917	0.8769735251
H	-0.8074781501	-3.1827135094	1.4406963446
C	-2.5297099234	-2.7769429028	0.1999000906
H	-1.4525426679	-1.5548758331	1.6119616478
H	-2.9860772401	-1.9132209257	-0.2994594832

H	-3.2398512635	-3.0893144151	0.9763859233
C	-2.3557347334	-3.9141549186	-0.8125587308
H	-1.7333788448	-3.60805114	-1.6600200838
H	-3.3209724264	-4.2388733975	-1.2145798075
H	-1.8764024224	-4.784615105	-0.34942516
C	-3.2013905436	1.3944063774	-0.750627854
H	-1.4786703145	1.6986979982	-2.0003568217
H	-1.4585433669	2.656582342	-0.5309853621
H	-3.7275795725	2.0112801326	-1.4913864291
C	-3.7971665836	1.7150225004	0.630172107
H	-3.4176715018	0.3504169677	-1.0127790976
C	-3.3975361572	0.7688366555	1.7680921371
H	-4.8910762774	1.7016371544	0.5372029366
H	-3.5319231918	2.7466617967	0.9006888933
H	-2.332191774	0.8357245452	2.0023355483
H	-3.6116408476	-0.2726209676	1.5055861976
H	-3.9512673439	1.0042629647	2.6833168748
C	3.1472296414	0.8888693604	0.7929187874
C	4.1416230698	-0.2864788087	0.8109083149
H	4.7654563219	-0.3020902138	-0.0887111311
H	4.8077172201	-0.1940333265	1.674959109
H	3.6304749282	-1.2513984043	0.8907986052
C	3.9606550659	2.2036923815	0.7743836466
H	3.3061380565	3.0797557396	0.8011314009
H	4.6311378679	2.2568803295	1.6400355239
H	4.5692702313	2.2701640089	-0.1334548247
C	2.3110412211	0.8271787179	2.0921600829
H	2.9659222575	0.8652405014	2.9701935682
H	1.6096750005	1.6631709828	2.1672973278
H	1.7323245305	-0.1009581014	2.1413889932
H	1.7323245305	-0.1009581014	2.1413889932

TS exo 0370

E(RB3LYP) = -706.412057610 A.U.

First frequency = -510.9141 cm^{-1}

H	1.077440944	-1.0066026239	-3.078602084
C	1.0228833176	-0.2225328697	-2.3275257238

H	0.3619816607	0.5960094215	-2.5933483938
C	2.1115019553	-0.0170390502	-1.4917510269
C	2.0750974962	0.8839294114	-0.4033561826
C	0.9354085304	1.6559368229	-0.2367826923
H	0.8193452699	2.2993251692	0.6253893086
H	0.3577303269	1.9628740175	-1.0986597446
C	-0.8367634405	0.1348200343	-0.0921031462
H	-0.5767195137	0.0354911144	0.958842725
C	-1.9966589988	1.0570093889	-0.4136091089
C	-0.5172695368	-0.9239639513	-0.9439799829
H	-1.174179001	-1.0692104561	-1.8004483758
C	0.1310561653	-2.1746856396	-0.3859752394
H	2.9217170268	-0.740591466	-1.5362332904
H	1.006088057	-1.8796663544	0.2028463322
H	0.506501101	-2.7995661712	-1.2060910839
C	-0.8078917148	-3.0141811829	0.5017740196
H	-0.2416088118	-3.8589209762	0.9189260561
C	-2.0442456541	-3.5515740638	-0.228007871
H	-1.1319492477	-2.4065540546	1.3577171374
H	-1.7224835686	-4.1308807453	-1.1048062855
H	-2.6303534389	-2.7094289895	-0.6173987906
C	-2.9321949727	-4.4204704821	0.6669759587
H	-3.8097038375	-4.7919082966	0.1274779436
H	-3.2892847852	-3.8535046333	1.5345106997
H	-2.3810583385	-5.2887218276	1.046345659
C	-2.2711075464	2.131575593	0.6452612129
H	-2.8995011706	0.4440551697	-0.5424859195
H	-1.833643889	1.5382498743	-1.390966557
H	-2.4489347484	1.639103782	1.6121556149
C	-3.4590187625	3.0497283824	0.3189159112
H	-1.3748293035	2.7470178992	0.7775568051
C	-4.8177561372	2.339846348	0.2905920315
H	-3.2804119055	3.5384674483	-0.648911005
H	-3.4939897909	3.8553380762	1.0632129052
H	-4.8700053872	1.5887103203	-0.5038878074
H	-5.6321096644	3.0519260672	0.1217980297
H	-5.0122423381	1.8295127456	1.241221411
C	3.2063152286	0.8371585681	0.6452753125

C	3.0168348513	1.8864214016	1.7562065678
H	3.8613932547	1.8474869312	2.4520415717
H	2.9652870219	2.9007591989	1.3478530113
H	2.1058805479	1.7039645398	2.3357707886
C	3.2749221744	-0.5552367922	1.3141556654
H	4.0947106465	-0.5930065453	2.040932201
H	2.34318843	-0.7763881028	1.8452490313
H	3.4418818773	-1.3506504277	0.5824471285
C	4.5494145905	1.1280294562	-0.063476581
H	4.5334554682	2.1159966372	-0.5348634022
H	5.3749577978	1.1056735864	0.6572299259
H	4.7669979498	0.3909067963	-0.8417117682
H	4.7669979498	0.3909067963	-0.8417117682

TS exo 0371

E(RB3LYP) = -706.411808155 A.U.

First frequency = -501.6802 cm⁻¹

H	1.4533938195	-0.7543449696	-3.383249536
C	1.3678727227	-0.0095548062	-2.5963574293
H	0.8531164823	0.8955889839	-2.8960912067
C	2.2885978382	-0.0144942094	-1.5596112972
C	2.1572698286	0.8182570641	-0.4271555693
C	1.1091847011	1.7302549925	-0.4203865854
H	0.8986763945	2.3279176683	0.4614932892
H	0.7795499271	2.1851403671	-1.3454813344
C	-0.7765082284	0.4865278379	-0.6171607637
H	-0.682267301	0.2925515038	0.4452960887
C	-1.7352352699	1.5881910362	-1.0272448239
C	-0.5089371521	-0.5764094208	-1.4838129508
H	-1.0318528291	-0.5783246922	-2.440182432
C	-0.0915334334	-1.9379747066	-0.9685378212
H	2.9853172408	-0.8447793251	-1.5213870294
H	0.6066843341	-1.8013886124	-0.1327123404
H	0.4685021443	-2.4680339831	-1.746866229
C	-1.2557509835	-2.8436943036	-0.5146018123
H	-1.9822643341	-2.9375807507	-1.3344227471
C	-1.9824183849	-2.383686419	0.7528111006

H	-0.8582395932	-3.8546035359	-0.3462106969
H	-2.4274585565	-1.399899171	0.5777823569
H	-1.2487184204	-2.2459978072	1.5596513615
C	-3.0699239037	-3.3624842551	1.2041449841
H	-3.8290124438	-3.4928936705	0.42412216
H	-3.5785851675	-3.0097710015	2.1075259705
H	-2.6493266746	-4.3509746135	1.4218903793
C	-3.2159181755	1.3336758357	-0.6431789444
H	-1.6628819018	1.7079424212	-2.1161344001
H	-1.4339198019	2.5531824911	-0.5992836319
H	-3.861074949	1.7958903584	-1.4012718281
C	-3.6278982404	1.8990313374	0.7267820302
H	-3.4227143497	0.2571438072	-0.6849380365
C	-2.8300861927	1.3758534787	1.9264313468
H	-4.6934571991	1.6879575348	0.8851315289
H	-3.5383618314	2.9937187135	0.6920626522
H	-2.8827825495	0.2847543836	1.998768903
H	-3.216974131	1.7911500746	2.8629046098
H	-1.7731495223	1.6531923058	1.8584352022
C	2.9732244548	0.5882926849	0.8619481053
C	3.7179710215	1.8927276802	1.2287191006
H	3.0207562001	2.720392423	1.388524344
H	4.3012473036	1.7609112303	2.1475164719
H	4.4045124578	2.1854512143	0.42747875
C	2.0245298352	0.202313113	2.0207453523
H	1.2780089728	0.9779736324	2.2147185809
H	1.4905271702	-0.7268063945	1.7964114024
H	2.5926889041	0.0515998224	2.9457949604
C	4.0189327093	-0.5313851119	0.7095638631
H	4.7214518226	-0.3200250185	-0.1032015832
H	4.5986730233	-0.6246412327	1.6337031011
H	3.5509365921	-1.5017574238	0.5147117986
H	3.5509365921	-1.5017574238	0.5147117986

TS exo 0372

E(RB3LYP) = -706.413050338 A.U.

First frequency = -502.4034 cm⁻¹

H	0.6630270161	-0.5069707188	-3.2849529269
C	0.8108842399	0.1286398893	-2.4160629906
H	0.4953892696	1.1557706338	-2.559485142
C	1.8083603879	-0.1917344912	-1.5075497847
C	1.9787903241	0.5046728745	-0.2892596058
C	1.1316619554	1.573543093	-0.0365420893
H	1.1470889142	2.0798854344	0.9234814375
H	0.7654656961	2.1859964472	-0.8494669055
C	-1.0054811316	0.7069985479	-0.1555440105
H	-0.8636601429	0.2731976174	0.8294768619
C	-1.7264635673	2.0379641514	-0.1814066187
C	-1.0820036392	-0.1518222657	-1.2526294183
H	-1.6256417286	0.2356461957	-2.1149294113
C	-1.1428532221	-1.6672312487	-1.1329361401
H	2.3220080257	-1.1369778693	-1.6474138746
H	-0.7653224893	-2.1254753569	-2.0554448219
H	-2.2040007488	-1.9586008829	-1.0731022555
C	-0.4015052517	-2.2762676623	0.059933239
H	0.6315354698	-1.9171884994	0.0569522714
C	-0.4026277926	-3.8079253357	0.0549395961
H	-0.8483539053	-1.9219336275	0.9983980186
H	0.0490241927	-4.1663493405	-0.8802025269
H	-1.4381815148	-4.174853635	0.0522908267
C	0.3529888967	-4.3992485862	1.2486729582
H	0.3494860127	-5.493922648	1.2290629213
H	-0.0962258925	-4.0803734848	2.1962899894
H	1.3981880345	-4.0682630799	1.2541603543
C	-3.2302917166	1.8987399398	0.1158328047
H	-1.602749317	2.5046081523	-1.1696050994
H	-1.2855654397	2.7331823631	0.5440985808
H	-3.6813407739	1.2263141359	-0.6263307118
C	-3.9736696742	3.2391214892	0.1173593833
H	-3.3614946717	1.4063366414	1.089706984
C	-5.4694470529	3.0924816793	0.4111650306
H	-3.8353838956	3.7294602328	-0.8560966456
H	-3.5155721393	3.9061221217	0.86044093
H	-5.6345265167	2.6337789909	1.3928024232
H	-5.9566105348	2.4552146514	-0.3357000386

H	-5.9785686495	4.0618417488	0.405922359
C	2.9321181058	0.005617606	0.8183884048
C	2.157016203	-0.249505607	2.1317944123
H	2.844783812	-0.5839528471	2.9166658021
H	1.6596901749	0.6537872964	2.495857829
H	1.3949912022	-1.0221089042	1.9984346256
C	3.6627558596	-1.2952620063	0.4353608278
H	4.2532020053	-1.1745512229	-0.4785931729
H	4.350928382	-1.5811919328	1.2374814931
H	2.9679333635	-2.1283017173	0.2865141397
C	3.9999188106	1.0966182971	1.069019954
H	4.5746768905	1.2941784394	0.1581042475
H	3.5382125028	2.0377570238	1.3822463374
H	4.6987962112	0.7832572529	1.8535164208
H	4.6987962112	0.7832572529	1.8535164208

TS exo 0375

E(RB3LYP) = -706.413370119 A.U.

First frequency = -487.2807 cm⁻¹

H	1.3793170425	-0.7365907557	-3.3906849004
C	1.1894640175	-0.034881299	-2.5827588766
H	0.675387602	0.868510368	-2.8894956599
C	1.9917859461	-0.0721238093	-1.4543976913
C	1.714227437	0.6968880133	-0.3011935764
C	0.6706610289	1.6088416877	-0.3651622793
H	0.3710155127	2.1650426123	0.5163880952
H	0.426716138	2.0956824205	-1.3004833705
C	-1.2001735644	0.3331797514	-0.848640798
H	-1.2281669928	0.1131504697	0.2139239557
C	-2.1683535867	1.3883768395	-1.3474609175
C	-0.777948077	-0.6928143934	-1.6911373669
H	-1.1818086242	-0.7113598345	-2.7024911306
C	-0.3614169493	-2.0204143319	-1.1010657375
H	2.7029290347	-0.8875584695	-1.381287151
H	0.3670114895	-1.8219122683	-0.3070106484
H	0.1620885768	-2.6257648387	-1.8516131268
C	-1.5365215231	-2.8320089456	-0.5263661819

H	-2.0582961129	-2.2250956679	0.2259706829
C	-1.1154311252	-4.1692979049	0.1029881
H	-2.2665095709	-3.0192951477	-1.3249322625
H	-0.594575653	-4.7767967321	-0.6499488005
H	-2.017481254	-4.7313902064	0.3766396114
C	-0.2254599321	-4.0192414235	1.3431707359
H	-0.7127481239	-3.3938406715	2.1007510365
H	0.7359433095	-3.5542132635	1.1022443894
H	-0.013217129	-4.991401151	1.7999568279
C	-2.3842227405	2.6231157412	-0.456233149
H	-3.1473562274	0.9041987556	-1.4898070252
H	-1.8569401253	1.7153832835	-2.3496846611
H	-1.4795971422	3.2413563531	-0.4331845601
C	-2.8082272376	2.301917084	0.9821174721
H	-3.1600899088	3.246496487	-0.9209835612
C	-3.1225880058	3.5591931556	1.7980487896
H	-2.0128910582	1.7374527563	1.4846885221
H	-3.6861960781	1.6415352005	0.9635154337
H	-3.9409183894	4.1300511215	1.3445870031
H	-2.250265274	4.2210024879	1.8508264953
H	-3.4155305171	3.3117958753	2.8235306925
C	2.3848381076	0.4077445345	1.0592436709
C	3.1085372598	1.6844897836	1.5458646942
H	3.5906156263	1.512176508	2.5152611764
H	3.8793304328	1.9896420163	0.8304694321
H	2.4109254528	2.5194878669	1.6597698075
C	1.3141132392	0.0037046515	2.0999506789
H	1.7812840027	-0.1829144665	3.0736435832
H	0.5626264988	0.7861025492	2.2402258676
H	0.7941262319	-0.9101666947	1.7952830884
C	3.4199385628	-0.7293809513	0.9812337639
H	3.8858938211	-0.8734986885	1.9614585509
H	2.9585194366	-1.6795563968	0.6920998016
H	4.2171757957	-0.503748434	0.2655969382
H	4.2171757957	-0.503748434	0.2655969382

TS exo 0381

E(RB3LYP) = -706.412297341 A.U.

First frequency = $-522.7273 \text{ cm}^{-1}$

H	0.3196623984	-0.2526891147	-3.1522535082
C	0.4062978983	0.3207062015	-2.2329278818
H	-0.1970668079	1.2196169274	-2.2137428218
C	1.567356073	0.2184515297	-1.4815932207
C	1.7017287899	0.8004762202	-0.2012010186
C	0.6434852011	1.5657096461	0.2716430498
H	0.6399438692	1.9600768612	1.2806815754
H	0.0478707148	2.1426009814	-0.4237495191
C	-1.159680003	0.1942862289	0.2855323384
H	-0.7567694768	-0.2507761354	1.1927093697
C	-2.2423014978	1.2300746514	0.5386319203
C	-1.0978365015	-0.5965827899	-0.8655761508
H	-1.8576722028	-0.4457905829	-1.6287403066
C	-0.531619042	-1.9969796571	-0.7690236326
H	2.2943632648	-0.5316185499	-1.7836900697
H	0.4183220895	-1.9453057749	-0.2282625368
H	-0.2964478332	-2.3857427961	-1.767872883
C	-1.4775730434	-2.9809821818	-0.0572378122
H	-1.7041201191	-2.597682484	0.9471601556
C	-0.9181929332	-4.4078102846	0.0559893929
H	-2.4347906073	-3.0073629145	-0.5949908641
H	-0.6886983651	-4.7875054108	-0.949275575
H	-1.7003745094	-5.064515379	0.4579573892
C	0.3296805743	-4.5172437068	0.9408699168
H	0.1306248965	-4.127669359	1.9463870713
H	1.1720872768	-3.9514173588	0.5308185601
H	0.6523736058	-5.5583548598	1.0450286575
C	-2.7837655683	1.9603988936	-0.6984142717
H	-1.8716452316	1.9653939525	1.2621173096
H	-3.0875097647	0.7301819451	1.0383313146
H	-1.9585732834	2.4411920188	-1.2410303437
C	-3.8478389919	3.021251361	-0.3736681219
H	-3.2174351936	1.2287139866	-1.3903400205
C	-3.3131426065	4.2299321472	0.4034909743
H	-4.6642163287	2.5516196306	0.192123572
H	-4.2919806455	3.3717574989	-1.3138127649

H	-2.9392965863	3.9479009521	1.3927308116
H	-4.0951207866	4.9817954706	0.551173961
H	-2.4880950808	4.7081026836	-0.1374553881
C	2.8920319295	0.3865908604	0.6888898199
C	4.2058525652	0.7417670957	-0.0445124464
H	5.0724948879	0.4605057239	0.56483117
H	4.2900269588	0.2217579225	-1.0030610533
H	4.2611358888	1.8170814288	-0.2424812315
C	2.8890065788	1.119019402	2.0433546695
H	2.0104863092	0.8597080234	2.6433084171
H	3.7750430669	0.8363784504	2.6213744175
H	2.9054386847	2.205780101	1.9129900103
C	2.8619238324	-1.134081667	0.9711997694
H	2.8994496322	-1.7195706544	0.0480821032
H	3.7191846753	-1.4284536719	1.5877119342
H	1.9494598116	-1.4127251736	1.5084957643
H	1.9494598116	-1.4127251736	1.5084957643

TS exo 0388

E(RB3LYP) = -706.411850702 A.U.

First frequency = -511.8781 cm^{-1}

H	0.5225588899	-0.8918319377	-3.0959250437
C	0.552339445	-0.1460385704	-2.3053900308
H	-0.0467117407	0.7353196192	-2.5103194482
C	1.6777828729	-0.0712234938	-1.4964799381
C	1.7449822245	0.7728174493	-0.3650167016
C	0.6775339592	1.6246166066	-0.1259904948
H	0.6342303657	2.2280139214	0.7711227084
H	0.1036336865	2.0208210565	-0.9534143624
C	-1.2095723014	0.2408289359	-0.0037124193
H	-0.933007653	0.0728259748	1.0343468699
C	-2.2977508017	1.2647335072	-0.2552887944
C	-0.9930306404	-0.7988927393	-0.9097920455
H	-1.6859475132	-0.8636322951	-1.7489958673
C	-0.4280887453	-2.1175025918	-0.4276040623
H	2.4242996039	-0.8545451897	-1.6018591227
H	0.441194957	-1.916875279	0.2096168364

H	-0.0575156479	-2.6974852592	-1.2796048746
C	-1.4489426632	-2.9506420536	0.3685858843
H	-1.8367650885	-2.3354835399	1.190382753
C	-0.8777402758	-4.2572572055	0.9413383077
H	-2.3118756131	-3.179516473	-0.2731445001
H	-1.6330214885	-4.7174251871	1.5913502861
H	-0.0217644193	-4.0204715042	1.58852021
C	-0.4472816335	-5.2750053944	-0.1213174878
H	-0.1116843284	-6.2102530327	0.3386935942
H	0.3764103975	-4.8978756108	-0.7356996822
H	-1.2793422987	-5.5138594424	-0.7941832946
C	-2.4198503207	2.3560494962	0.8159684881
H	-3.2651984249	0.7425228778	-0.3223908853
H	-2.1472889939	1.7186741055	-1.2454426405
H	-2.4806347057	1.8717504374	1.8000001612
C	-3.6366800729	3.2756181746	0.6338299318
H	-1.5102981742	2.9678348336	0.8318477185
C	-3.589930947	4.1232189812	-0.6429468862
H	-3.7081738073	3.9418602792	1.5028500243
H	-4.5532008237	2.6696284888	0.6379252665
H	-2.6732327821	4.7235540353	-0.6805666493
H	-4.4408520591	4.8101765363	-0.6942981935
H	-3.6150136267	3.5024222607	-1.5442747588
C	2.8955882239	0.5800094498	0.6452193591
C	2.825406814	1.5855571452	1.809163303
H	2.847976096	2.6194140482	1.4501261276
H	1.9184779769	1.4508309252	2.4077588201
H	3.6822620978	1.4429931373	2.4758825399
C	2.8640354236	-0.8444756788	1.2459274174
H	3.6997240281	-0.9875613093	1.9408016377
H	1.9338446863	-1.0113665425	1.7991221093
H	2.9378068745	-1.6143609951	0.4728077053
C	4.2392720463	0.7923957993	-0.0897853834
H	5.078701486	0.6669990499	0.6038322238
H	4.3737068658	0.07822062	-0.9072231866
H	4.2940109442	1.7998908715	-0.5146177006
H	4.2940109442	1.7998908715	-0.5146177006

TS exo 0390

E(RB3LYP) = -706.412380113 A.U.

First frequency = -503.0512 cm⁻¹

H	1.3745741933	-0.9242651093	-3.1027742023
C	1.1658782966	-0.1430681383	-2.3763205975
H	0.6490919904	0.716471883	-2.7887170105
C	1.9859781878	-0.0199779861	-1.2650121457
C	1.7003536832	0.8717871294	-0.205883368
C	0.6082610809	1.7137050765	-0.3451370588
H	0.2933492441	2.3608367346	0.4626334008
H	0.311064172	2.056309624	-1.3278526759
C	-1.2030834483	0.2897063384	-0.6689201077
H	-1.1967630657	0.1211140015	0.4038508748
C	-2.2427572614	1.2611661318	-1.1941566806
C	-0.7504928768	-0.7584438658	-1.4728733463
H	-1.1783091454	-0.8268220804	-2.473375513
C	-0.3465514285	-2.0746885687	-0.8435648778
H	2.7282700616	-0.7970939775	-1.1002955025
H	0.3209971958	-1.8721489537	0.0024509476
H	0.2336381799	-2.6681655072	-1.5582099501
C	-1.551645464	-2.8915566045	-0.3422162212
H	-2.1390457955	-2.2642185745	0.34030576
C	-1.1680796013	-4.1957101962	0.3744643501
H	-2.2136765037	-3.1212651286	-1.1894416552
H	-2.0742645846	-4.6422056522	0.8036647626
H	-0.5133124958	-3.9579223095	1.2243827117
C	-0.4807201077	-5.2294471535	-0.5251372019
H	-1.1055997878	-5.4697161336	-1.3934206991
H	-0.2901839778	-6.1617852481	0.0165122575
H	0.4810458566	-4.8662219983	-0.9008836094
C	-2.4894408543	2.5454300881	-0.384498666
H	-3.200042401	0.7197532834	-1.259218936
H	-1.9906062175	1.529780668	-2.2298737575
H	-1.6257513251	3.2158713254	-0.4575436413
C	-2.8185730247	2.3107835149	1.0946199872
H	-3.3255850902	3.0846078668	-0.8501318491
C	-3.1698176929	3.6059173784	1.8325886873

H	-1.9638630695	1.835141936	1.5914410098
H	-3.6527645929	1.5999453233	1.1733890915
H	-3.3938351068	3.4207225133	2.8881373484
H	-4.0446311523	4.0911009319	1.3848290786
H	-2.3393630787	4.3201244727	1.7883241714
C	2.4742358836	0.7328812535	1.1213221735
C	2.2449670734	-0.6656903436	1.7403290854
H	1.1852247163	-0.8190283639	1.9699155996
H	2.5613681549	-1.465933025	1.065516393
H	2.8111138088	-0.7716482684	2.6730442268
C	3.982239145	0.9243090447	0.8397245645
H	4.1748422492	1.9144273742	0.4141627299
H	4.5594869386	0.831724931	1.7668844196
H	4.3625420482	0.1790275059	0.1352610507
C	2.0452819715	1.7857772477	2.159921042
H	2.6480057139	1.679659862	3.0679075044
H	2.1836801625	2.8038374464	1.7822125376
H	0.9953450085	1.6678478689	2.4481139042
H	0.9953450085	1.6678478689	2.4481139042

TS exo 0400

E(RB3LYP) = -706.412315984 A.U.

First frequency = -524.4960 cm^{-1}

H	1.4785347347	-0.288711715	-3.3765889886
C	1.3450909553	0.3355087899	-2.4966460124
H	0.8429848943	1.2755570246	-2.6966215483
C	2.2397978871	0.2117208102	-1.4417986055
C	2.0537639627	0.8743441594	-0.2094806211
C	0.9727870751	1.741207625	-0.1098013106
H	0.7091116662	2.211127219	0.8303492948
H	0.6616296176	2.3044755681	-0.9802628911
C	-0.8658061726	0.5084935263	-0.5817082123
H	-0.8271076499	0.1469621601	0.4395112536
C	-1.8225439386	1.6519376406	-0.864115082
C	-0.5305275071	-0.3990911848	-1.5954057499
H	-1.0234580872	-0.2558505373	-2.5577224738
C	-0.1356841712	-1.8287669668	-1.2831522775

H	2.9599858717	-0.6015598958	-1.4879783866
H	0.4933693599	-1.8364120453	-0.3874235416
H	0.492525444	-2.2205691844	-2.0909597033
C	-1.3222541456	-2.8007368492	-1.1037924384
H	-1.9407557004	-2.7691564154	-2.011136736
C	-2.2204564138	-2.5590904699	0.1177687293
H	-0.9185716903	-3.8215944185	-1.0461835725
H	-3.0471674598	-3.2804441406	0.0880994961
H	-2.6781311022	-1.5678982225	0.0402746772
C	-1.4984901184	-2.6831012379	1.4634715311
H	-1.0041951212	-3.6570045651	1.558167166
H	-2.1979206725	-2.5805560766	2.2997110002
H	-0.730486265	-1.9127782316	1.5856807952
C	-3.3210777828	1.3244204443	-0.6405928038
H	-1.6770117146	1.9586265766	-1.9083828488
H	-1.5735841152	2.5318098101	-0.2566370936
H	-3.9188332184	1.9187006539	-1.3436435902
C	-3.8379289343	1.6230566558	0.7771435907
H	-3.5071376819	0.2746265271	-0.8977250605
C	-3.1148948876	0.8933412936	1.9147687673
H	-4.9073639853	1.3785116511	0.8166728983
H	-3.7688594626	2.7059023501	0.9509879261
H	-3.5776564619	1.1220488755	2.8805450881
H	-2.063176504	1.1904244453	1.9788229385
H	-3.1451807205	-0.1922298679	1.7793873677
C	2.8975423156	0.4499264999	1.0095481751
C	2.6561574745	-1.0392358806	1.3490065206
H	3.2790545118	-1.3470985227	2.1968729556
H	1.6096981994	-1.2102680948	1.6222030992
H	2.8935843133	-1.69284333	0.50511196
C	4.3921391784	0.6598184471	0.6745532994
H	5.0194750485	0.3684405717	1.5248376455
H	4.7030712687	0.063700547	-0.1881958855
H	4.5943871959	1.7107985288	0.4441935719
C	2.5674172974	1.2808588916	2.263182438
H	3.2205679452	0.9829149272	3.0900197586
H	2.7149701486	2.3511226364	2.0869539497
H	1.5338976207	1.1275379597	2.591125551

H 1.5338976207 1.1275379597 2.591125551

TS exo 0404

E(RB3LYP) = -706.412787303 A.U.

First frequency = -492.2244 cm^{-1}

H	1.3003157395	-0.1297864403	-3.4693524472
C	1.2556043232	0.4562064276	-2.55524682
H	0.8002722467	1.4324660432	-2.6740934622
C	2.1602564213	0.1933970557	-1.5393244383
C	2.0737062149	0.8047752793	-0.2684004134
C	1.0965999206	1.7744206669	-0.0851795835
H	0.9234446665	2.2095836596	0.8943093727
H	0.8036596397	2.4152842467	-0.9065306466
C	-0.8738356948	0.7139174101	-0.5089886329
H	-0.7986929904	0.3243932326	0.5007140907
C	-1.7376295282	1.9444756838	-0.6926666717
C	-0.6774576768	-0.1753267678	-1.5653176884
H	-1.1867696724	0.0596757098	-2.4998165845
C	-0.3757855438	-1.6424333576	-1.3444705336
H	2.8003081625	-0.6736994358	-1.6605296759
H	0.4417768444	-1.7317275428	-0.6195210252
H	0.0055603791	-2.0705640718	-2.2777262215
C	-1.5935749834	-2.4754441705	-0.8670061918
H	-2.5017063729	-2.0772244119	-1.3366949561
C	-1.7821086363	-2.5303342338	0.6586886908
H	-1.489222697	-3.5053784103	-1.235067254
H	-2.7852747492	-2.9150583534	0.882466572
H	-1.7494272453	-1.5162771401	1.0727573342
C	-0.7444572723	-3.406920258	1.3692383423
H	-0.8098273806	-4.4456542364	1.0254733873
H	-0.8937377659	-3.4024507607	2.4538779766
H	0.2779093999	-3.0644092567	1.1780072527
C	-3.2512775174	1.6461879882	-0.7516203183
H	-1.4534481924	2.4474836295	-1.6275090487
H	-1.539928264	2.6645420264	0.1094117414
H	-3.7880513342	2.5988272824	-0.8628829215
C	-3.8117540389	0.8890124537	0.4618351225

H	-3.4592620539	1.0624107948	-1.657353003
C	-3.5524037891	1.5784330518	1.8053648033
H	-3.3862983598	-0.120644546	0.483681932
H	-4.8926162801	0.759922028	0.3229853669
H	-4.0394331591	1.0418864435	2.6260220503
H	-3.9345074923	2.6060874784	1.804172962
H	-2.4822620818	1.6254050206	2.0340299282
C	2.8601129811	0.2799699157	0.9511765281
C	3.7878936769	-0.8967959653	0.5979152031
H	4.3469577392	-1.2069119956	1.4867466216
H	3.2247378407	-1.7659938644	0.2422787634
H	4.5161802833	-0.6217170314	-0.1718737148
C	3.7299560092	1.4243906549	1.520409248
H	4.4460574288	1.776943401	0.7707714535
H	3.1167088329	2.2784574024	1.8226628798
H	4.2927692162	1.0847228065	2.3977519952
C	1.8757857692	-0.2010344329	2.0423906023
H	2.424650158	-0.5807069437	2.9116243441
H	1.2237929343	0.6047064486	2.3916066465
H	1.2382043731	-1.00668983	1.6658261018
H	1.2382043731	-1.00668983	1.6658261018

TS exo 0405

E(RB3LYP) = -706.412609831 A.U.

First frequency = -516.3582 cm⁻¹

H	0.9674283706	-0.2745410694	-3.3896730414
C	0.8668066707	0.2653014155	-2.4512929245
H	0.1905724633	1.1125948417	-2.5034470397
C	1.9266598881	0.2533484246	-1.5540744644
C	1.8299955534	0.8134245178	-0.2611241443
C	0.6623309211	1.4848675924	0.0690700883
H	0.4962269846	1.8552873075	1.0720703106
H	0.1052144302	2.012207091	-0.6943985051
C	-1.0503587572	-0.0602347848	-0.2823729045
H	-0.8118545186	-0.4309416081	0.7095674295
C	-2.2334301597	0.8820543675	-0.3820069995
C	-0.674362256	-0.8381540623	-1.3813110174

H	-1.312077094	-0.7618311136	-2.2632394163
C	-0.009094607	-2.1856860339	-1.1915538024
H	2.7585357917	-0.4127552732	-1.7689339652
H	0.7226681749	-2.1109073597	-0.3810301394
H	0.5634058852	-2.4473664795	-2.0888498708
C	-0.9998922754	-3.3365727153	-0.9081149889
H	-1.7165957422	-3.3921506234	-1.7388101242
C	-1.7776348991	-3.2509635687	0.4142240543
H	-0.4397737239	-4.2822449474	-0.9255676337
H	-2.4933731404	-4.0823516281	0.4485623022
H	-2.3760096331	-2.3323779536	0.4288450489
C	-0.891656064	-3.3063093865	1.6635676829
H	-0.2715388174	-4.2103883626	1.666599329
H	-1.494554115	-3.3113763327	2.5775556912
H	-0.2152089903	-2.447452823	1.7225365424
C	-2.5481704721	1.6571365455	0.9038182136
H	-3.1273508395	0.3004657971	-0.6571646761
H	-2.0756378665	1.5785255053	-1.2181695405
H	-2.6116007455	0.9404645446	1.7338940791
C	-3.8510221808	2.4681210132	0.8410392119
H	-1.7191106903	2.3325525425	1.1455395497
C	-3.8273666619	3.6042597679	-0.1881955538
H	-4.0521102179	2.8893407091	1.8341729398
H	-4.6888070576	1.7920476623	0.6212591912
H	-2.986557504	4.2829779165	-0.0023840704
H	-4.7481678442	4.1951112084	-0.1478794566
H	-3.7257136932	3.2250292911	-1.2100871467
C	2.9217777613	0.4871482518	0.7793676989
C	2.672300966	1.1882867459	2.1273551873
H	3.4919665354	0.9670066772	2.8188948655
H	2.6149320617	2.2752793028	2.011342789
H	1.7451460005	0.8449519459	2.5980017388
C	2.9866523647	-1.0354888505	1.0408228219
H	3.7839191305	-1.2699596308	1.7556820061
H	2.0423204481	-1.3974406865	1.4608921854
H	3.1835188337	-1.5981890966	0.1241281029
C	4.2860752654	0.9690943633	0.2345883099
H	5.0832549993	0.7541610689	0.9554918849

H	4.5465469906	0.4755333215	-0.7060452144
H	4.2715405336	2.0484671154	0.0521461568
H	4.2715405336	2.0484671154	0.0521461568

TS exo 0407

E(RB3LYP) = -706.413564203 A.U.

First frequency = -492.0512 cm⁻¹

H	0.8054134454	-0.9438478878	-3.0959548143
C	0.8713473485	-0.1454522024	-2.3628936713
H	0.4376539778	0.7921577177	-2.6883314557
C	1.8465530463	-0.2020178228	-1.383147758
C	1.9176441416	0.7311727788	-0.3237034945
C	1.0318856314	1.8033747444	-0.3523627891
H	0.9866999679	2.504333262	0.4758286531
H	0.7365143991	2.2322859839	-1.3014545378
C	-1.0343160468	0.9185825955	-0.3379367904
H	-0.9468991203	0.8822490243	0.7449741688
C	-1.8100028065	2.0897990908	-0.9011827122
C	-0.9982836432	-0.3013923137	-1.0097139785
H	-1.5612959282	-0.3966077623	-1.9365299103
C	-0.7203677652	-1.5684440648	-0.2358623869
H	2.4267767396	-1.1162067539	-1.3169756755
H	-1.4696541645	-1.6602516231	0.5631504854
H	0.245357519	-1.454662495	0.2782186773
C	-0.7050436007	-2.8505629161	-1.0723735845
H	-1.690096517	-2.9893364466	-1.5409375218
C	-0.3366597797	-4.1120618031	-0.2771498182
H	0.0102497247	-2.7279236261	-1.8931110108
H	0.6567266077	-3.9728714428	0.1721275144
H	-0.2389582148	-4.9531729396	-0.9752609682
C	-1.3434658963	-4.4861252445	0.8167980165
H	-1.0672961816	-5.4268069706	1.3043522465
H	-2.3488486556	-4.610067951	0.3973583371
H	-1.4029093918	-3.7186137931	1.594971438
C	-3.3370346716	1.9570995178	-0.7157812698
H	-1.5981026854	2.1824297494	-1.9752725355
H	-1.4677012899	3.024801473	-0.4429850246

H	-3.8201152562	2.8533460574	-1.1296881515
C	-3.7935917184	1.7640220873	0.7389183736
H	-3.6897067746	1.1064355725	-1.3125384701
C	-3.3657963912	2.8933287252	1.6823482464
H	-3.4067705673	0.8084900264	1.1148197515
H	-4.8872198372	1.6756055084	0.7523685309
H	-2.2763764337	2.9448642042	1.782661802
H	-3.7807602412	2.750542745	2.6853286073
H	-3.7091375961	3.867220317	1.3139722228
C	2.7882069143	0.4921727499	0.9275700319
C	3.5861766807	-0.8224932262	0.8527723415
H	2.9267709472	-1.6952223229	0.7983139534
H	4.2540960991	-0.8428260152	-0.0144097164
H	4.2052804333	-0.9312006371	1.7492583486
C	3.7940817945	1.6586072603	1.0671164735
H	4.4265180552	1.5228030487	1.9522764772
H	4.4445329023	1.7170023197	0.1881956279
H	3.2786313331	2.6187389659	1.1642822517
C	1.8992511126	0.4372404007	2.1915730488
H	1.1850913602	-0.3901876328	2.1331987305
H	2.5169451852	0.2896761071	3.0847537529
H	1.3308334883	1.3606558513	2.3346428501
H	1.3308334883	1.3606558513	2.3346428501

TS exo 0413

E(RB3LYP) = -706.412078580 A.U.

First frequency = -514.7902 cm⁻¹

H	0.948642005	-1.4422035692	-2.6378475798
C	1.0325166438	-0.5091074327	-2.0879801032
H	0.5147114784	0.3244975393	-2.5483208815
C	2.1204612308	-0.3117267821	-1.2539780465
C	2.2394592034	0.8091429413	-0.400325255
C	1.2576647898	1.7895528602	-0.4889148648
H	1.2423363107	2.6333846239	0.190516522
H	0.8042612941	1.9973987547	-1.4497394388
C	-0.7033062642	0.7800094249	-0.0634010709
H	-0.4986614119	0.8886835321	0.9984928866

C	-1.6255396285	1.8178004821	-0.6723570226
C	-0.6638769233	-0.5144847683	-0.5830296002
H	-1.3126331453	-0.7321357602	-1.4273869338
C	-0.2852085933	-1.6808026832	0.3085522684
H	2.7864272262	-1.1559429805	-1.0913129329
H	-0.8377385049	-1.6061566239	1.257583838
H	0.7706316177	-1.5722014407	0.5810981524
C	-0.5323069057	-3.074036758	-0.2985733824
H	-0.3199330139	-3.0427010538	-1.3753025502
C	-1.9486332928	-3.6292660616	-0.0678221248
H	0.1835017768	-3.7860355694	0.130177712
H	-2.103430309	-3.7572162643	1.0124463744
H	-2.0068717546	-4.6351605518	-0.5036110115
C	-3.084787125	-2.7701466414	-0.6339382887
H	-3.1184784222	-1.7851801371	-0.1578141797
H	-4.0565375239	-3.2490964654	-0.4742099565
H	-2.9643765369	-2.6126831794	-1.7122435985
C	-3.1194052976	1.5449424382	-0.4039497365
H	-1.4697856832	1.8476266806	-1.75994687
H	-1.3676379894	2.8161060884	-0.2968618736
H	-3.7189595074	2.3199476925	-0.90175878
C	-3.4916089575	1.4971157731	1.0819898334
H	-3.3965169594	0.5912088154	-0.8727027744
C	-4.9841227366	1.2414714347	1.3089465235
H	-3.1984690707	2.4420769101	1.5603370406
H	-2.9077180558	0.7104446282	1.576044324
H	-5.5949871233	2.0263686253	0.8482776988
H	-5.230520716	1.2091877147	2.3752864363
H	-5.2885317372	0.2856009556	0.8670104976
C	3.3206870626	0.8067355196	0.6996179539
C	3.1375883945	-0.3980767922	1.6517221314
H	2.1645778967	-0.3540007732	2.1515219795
H	3.1984705157	-1.3507265578	1.118003497
H	3.9157210649	-0.3995853395	2.4238808488
C	4.7084967052	0.7129357185	0.0239270771
H	5.502901452	0.7104949608	0.7792308703
H	4.8096363807	-0.2003781265	-0.5695293147
H	4.8736533455	1.564643958	-0.6437845275

C	3.2887647534	2.0898693136	1.5500738698
H	4.0954096135	2.0656130638	2.2901375594
H	3.4255801886	2.9849664164	0.9350068304
H	2.3450616586	2.1908056049	2.0963320287
H	2.3450616586	2.1908056049	2.0963320287

TS exo 0434

E(RB3LYP) = -706.412944135 A.U.

First frequency = -522.7710 cm⁻¹

H	0.240569819	-1.3077594233	-2.7733151678
C	0.3140887143	-0.476851545	-2.0775183637
H	-0.2461059868	0.3997824925	-2.3846540242
C	1.4441425328	-0.3624558775	-1.2811475059
C	1.5683426191	0.620900011	-0.2742319922
C	0.5588482	1.5684902038	-0.1683961939
H	0.5548213699	2.2915807243	0.6370704388
H	0.0362094108	1.8967889811	-1.0572893977
C	-1.4281756726	0.3950605536	0.0917583213
H	-1.217625208	0.4243282539	1.1579718337
C	-2.4197028616	1.4172464474	-0.4256434385
C	-1.2618031243	-0.8248405272	-0.565249844
H	-1.9361616242	-1.0411484867	-1.3934105355
C	-0.7533382718	-2.0176121162	0.2143626325
H	2.1471980638	-1.1921468282	-1.2852174243
H	-1.4741509088	-2.2410668036	1.0161763711
H	0.1735642998	-1.7277397897	0.7233101117
C	-0.514715366	-3.2949495228	-0.594111232
H	-1.4319889838	-3.563184478	-1.1380792269
C	-0.075667238	-4.4770474342	0.2770851847
H	0.2504607154	-3.110916417	-1.3572065927
H	-0.8414951868	-4.6719734645	1.0401784002
H	0.8345737922	-4.1983372225	0.8258864078
C	0.1818818226	-5.7522123281	-0.530392454
H	0.4957373679	-6.5809757451	0.1126021
H	0.9680685114	-5.5929247984	-1.277404182
H	-0.7208684832	-6.068280776	-1.0657316243
C	-2.5180953362	2.7026603547	0.4030798829

H	-3.4179169944	0.9545656393	-0.464554452
H	-2.1820462301	1.6709303372	-1.4707973661
H	-2.7257096782	2.4388123538	1.4499567694
C	-3.6010171719	3.6624382989	-0.1014253915
H	-1.5525045829	3.2218483553	0.4068427135
C	-3.6954321412	4.945623132	0.7288165828
H	-4.5719654598	3.1485455423	-0.0979332695
H	-3.3965428554	3.9170697785	-1.1504736184
H	-2.7470535359	5.4948948226	0.7139408638
H	-3.9289614752	4.7207407341	1.7758221324
H	-4.4744774087	5.6148431027	0.3495448664
C	2.7259909743	0.5157023278	0.7414181681
C	4.060188835	0.6159510003	-0.0350753572
H	4.1230252547	1.5649055301	-0.5772647949
H	4.9104302797	0.5578641408	0.6543769193
H	4.1657564443	-0.192320549	-0.7645920055
C	2.6932896486	1.6489386953	1.783116908
H	3.5477252175	1.5551716007	2.4615063541
H	2.7488745917	2.6342165328	1.3095337246
H	1.7840556073	1.6127593783	2.3923919541
C	2.6859603024	-0.828606663	1.5039972332
H	1.7763319033	-0.9060114727	2.1082099121
H	2.7127754303	-1.6853720244	0.8247573837
H	3.5455517129	-0.9120877732	2.1790653362
H	3.5455517129	-0.9120877732	2.1790653362

TS exo 0437

E(RB3LYP) = -706.411803936 A.U.

First frequency = -501.8484 cm^{-1}

H	1.1158660102	-0.1148621365	-3.4304139459
C	1.0349323063	0.4217982789	-2.4884772058
H	0.3531985384	1.2649808803	-2.5179253306
C	2.0991594924	0.3810731861	-1.5994017617
C	2.0210564742	0.9338800127	-0.3022403577
C	0.8744052827	1.636515472	0.0389106504
H	0.7357886102	1.9992122652	1.0516449881
H	0.3236857239	2.1909004705	-0.7094391922

C	-0.8814303749	0.1217250324	-0.2929376345
H	-0.6436173533	-0.221042103	0.7094542694
C	-2.0425709596	1.0883286681	-0.4198869386
C	-0.5124835412	-0.6904946262	-1.3641958457
H	-1.139245557	-0.6420643581	-2.2550067128
C	0.182208985	-2.0153382379	-1.1334132969
H	2.9134877231	-0.2954682587	-1.8337897622
H	0.9108147874	-1.8950237614	-0.3215963827
H	0.7604510612	-2.292083528	-2.0222449754
C	-0.7727638817	-3.1790595687	-0.7945917609
H	-1.5070607078	-3.2905132645	-1.6052972752
C	-1.5146234531	-3.051495727	0.5407178052
H	-0.189029054	-4.1104080624	-0.7863341623
H	-2.1497406151	-2.158592569	0.5239619331
H	-0.7833154162	-2.8889971049	1.3450207998
C	-2.3682566447	-4.2820574231	0.8610074315
H	-2.8936032145	-4.1703703339	1.8152288293
H	-1.7526485148	-5.1869124994	0.9225725055
H	-3.1223963041	-4.450311521	0.0834182523
C	-2.3863288748	1.8339696185	0.8751117339
H	-2.9263169652	0.5297066989	-0.757364605
H	-1.8402785941	1.8177256174	-1.2202245757
H	-2.6120132523	1.0963579894	1.658726633
C	-3.5628993923	2.8133570598	0.7472005169
H	-1.5037031355	2.3836357648	1.2200404228
C	-4.9096648056	2.1461464285	0.4439638974
H	-3.3341695408	3.5499098381	-0.0355065789
H	-3.6494969037	3.3814989565	1.682041794
H	-4.9073058115	1.6450475474	-0.5292158471
H	-5.721044038	2.8811421423	0.431779566
H	-5.1526752912	1.3931300954	1.2028451933
C	3.0641549487	0.6103944757	0.7894443068
C	4.2168144507	-0.267048589	0.2676772237
H	4.9444316904	-0.4359985304	1.0682232975
H	3.8623047467	-1.2469172069	-0.0682480069
H	4.7444708439	0.210694392	-0.5642356715
C	3.6694462508	1.9318951188	1.3168559735
H	4.1634752979	2.4815324783	0.5088504559

H	2.8997933434	2.5836763987	1.7404711903
H	4.4116105078	1.7335152667	2.0989041728
C	2.3857549135	-0.1397319837	1.959018831
H	1.5784328385	0.4457503581	2.408032891
H	1.9610033975	-1.0902639195	1.6201635831
H	3.1152729039	-0.3570193752	2.7476175702
H	3.1152729039	-0.3570193752	2.7476175702

TS exo 0438

E(RB3LYP) = -706.413844464 A.U.

First frequency = -503.9778 cm^{-1}

H	0.3667541737	-0.9772577847	-3.068465148
C	0.3939760703	-0.2575068211	-2.2554301546
H	-0.1831712362	0.6406694566	-2.4426793903
C	1.4678499564	-0.2663696068	-1.3807027599
C	1.5151307903	0.5516270469	-0.2295562878
C	0.4980577261	1.4823366563	-0.0533200268
H	0.4501557749	2.0734797148	0.8551751084
H	0.0413614003	1.9572763346	-0.9119259409
C	-1.4806176089	0.2936427049	-0.0491349064
H	-1.3243692228	0.2023193599	1.0230326076
C	-2.4575803738	1.3626745069	-0.4960437473
C	-1.2660724283	-0.8414063221	-0.8267874035
H	-1.8819390703	-0.9758104388	-1.7146899805
C	-0.7155223623	-2.088947761	-0.1770509031
H	2.1722707453	-1.0861559595	-1.4717166473
H	-1.3994879877	-2.4044853418	0.6263638356
H	0.2228267568	-1.8190839817	0.3231383889
C	-0.487857283	-3.2732629721	-1.1207184107
H	-1.4244262088	-3.4903176174	-1.6522020827
C	-0.0028241218	-4.5471253709	-0.4124405426
H	0.2426875541	-2.9907820804	-1.8883428258
H	0.0305384568	-5.3664734538	-1.1416731838
H	-0.7389558449	-4.8446510403	0.3470001355
C	1.3765778119	-4.4052719537	0.2426292619
H	2.1260568516	-4.0828223334	-0.4899956014
H	1.7143936542	-5.3554258308	0.6689778404

H	1.368586182	-3.6675978441	1.051389525
C	-2.6165567894	2.538209804	0.4743517134
H	-3.4455334674	0.9006110422	-0.6442352105
H	-2.1670138937	1.7419785754	-1.4881026248
H	-2.8806414502	2.149193411	1.4681355029
C	-3.6785902112	3.5484827235	0.0274819754
H	-1.6578400362	3.0561240183	0.5963551436
C	-3.8335492815	4.7213050285	0.9997283189
H	-4.6427659341	3.0346869688	-0.0874150061
H	-3.4171099723	3.9289729888	-0.9695052814
H	-4.1243602037	4.370484568	1.9965601689
H	-4.5964128605	5.4289963054	0.6594249323
H	-2.8915739898	5.2714514902	1.1063818626
C	2.5463698006	0.325491629	0.8972529263
C	3.5150505963	-0.8318044898	0.59155602
H	4.078675604	-0.6551449076	-0.3302942404
H	4.2391076892	-0.932731102	1.4067021896
H	2.9903964738	-1.7875404038	0.4950980977
C	3.3807617695	1.6154710245	1.0758429992
H	4.12510453	1.4896397737	1.8708322691
H	3.9089152322	1.8665796467	0.1500910449
H	2.7464664612	2.4672201451	1.338698015
C	1.8245055841	0.0035260282	2.2259553261
H	1.2439259892	-0.9208134151	2.1438141817
H	2.5541611599	-0.126072166	3.0333810051
H	1.1401737711	0.8022471322	2.5258396402
H	1.1401737711	0.8022471322	2.5258396402

TS exo 0440

E(RB3LYP) = -706.413065498 A.U.

First frequency = -483.8548 cm^{-1}

H	0.5842505039	-1.2611136009	-2.7312402411
C	0.6915804513	-0.407982804	-2.0680763358
H	0.0473833975	0.4282352096	-2.3104734095
C	1.8633800368	-0.2459196823	-1.351641243
C	2.0286586795	0.7614627582	-0.3729046814
C	0.9954827213	1.6761703646	-0.2097575733

H	1.0316402139	2.4164414866	0.583796145
H	0.4003229935	1.9785113557	-1.0617737046
C	-0.8373452668	0.4652178749	0.3459687347
H	-0.4813685751	0.4954063075	1.3735376607
C	-1.9111189509	1.4708847265	-0.0059363086
C	-0.7669519741	-0.7584397756	-0.3138588186
H	-1.5143025697	-0.9590488414	-1.0774170269
C	-0.1337775412	-1.9445185886	0.3761998741
H	2.5840653055	-1.0555272066	-1.3963929601
H	-0.7283872956	-2.1813522407	1.2706245287
H	0.8492847321	-1.6338136725	0.7550028914
C	0.0370490999	-3.2215657028	-0.4610431522
H	0.8161898077	-3.0592808668	-1.2141723662
C	-1.2367078282	-3.721596266	-1.162262667
H	0.4101843223	-4.014374309	0.2012148573
H	-1.0018353553	-4.6584834317	-1.6831347135
H	-1.5287951911	-3.0116229077	-1.9466635633
C	-2.4209766077	-3.9483070539	-0.2164282116
H	-3.2772511956	-4.376041113	-0.7479225146
H	-2.751808264	-3.0106507338	0.2423562973
H	-2.1526197482	-4.6363833066	0.5937820617
C	-3.2741136094	1.1178666581	0.6196786456
H	-2.0254880115	1.5172871728	-1.0990832022
H	-1.6087466606	2.4739915093	0.3150718876
H	-3.5489572846	0.1046325799	0.300278545
C	-4.4066450717	2.0911738856	0.257749028
H	-3.16610789	1.0738988961	1.7127187665
C	-4.2158490922	3.5099693739	0.8064822674
H	-5.3528646101	1.6855705146	0.6380895607
H	-4.5106263073	2.1318766044	-0.8354231368
H	-4.0935423325	3.4948870401	1.895882818
H	-5.079398579	4.1426611936	0.5768173617
H	-3.3318311366	3.9960566364	0.3816193488
C	3.205579448	0.7524438458	0.6251885381
C	4.1809715547	-0.4137647816	0.3819018152
H	4.6079031691	-0.3814927064	-0.6257292414
H	5.0104312439	-0.3570808862	1.0943623876
H	3.6946201912	-1.3854300662	0.5173340651

C	3.9935848468	2.0754281543	0.4812925997
H	3.3573951794	2.9420738768	0.6840193581
H	4.8367682615	2.1034954515	1.1814199014
H	4.3890737381	2.182662656	-0.5341358745
C	2.67471638	0.6349728548	2.0725106912
H	2.0039884635	1.4590577933	2.3317427585
H	2.1251936742	-0.3012284518	2.2137405323
H	3.5066839365	0.6505304893	2.7858016666
H	3.5066839365	0.6505304893	2.7858016666

TS exo 0448

E(RB3LYP) = -706.412664987 A.U.

First frequency = -482.2818 cm^{-1}

H	1.3507068781	-1.5640421232	-2.857419756
C	1.1703405669	-0.6658897929	-2.2727259147
H	0.5340968986	0.0632494817	-2.760495995
C	2.0814096838	-0.3008047609	-1.2964251968
C	1.8427372876	0.7625390137	-0.3953585854
C	0.700559259	1.5270846318	-0.5790046706
H	0.4365145732	2.3010755311	0.1332087309
H	0.2956675838	1.6797322453	-1.5708505404
C	-1.0558387487	0.0149794719	-0.4065947416
H	-0.935638623	0.1014671879	0.668860427
C	-2.190115688	0.808412896	-1.0268367621
C	-0.6213212947	-1.1698953846	-0.994972529
H	-1.123557757	-1.4841630884	-1.9085828033
C	-0.0292961329	-2.2683545909	-0.1392246931
H	2.881853644	-1.0000153344	-1.0809886598
H	0.7622935575	-1.8371600081	0.4859912036
H	0.4600028267	-3.0157577919	-0.7734243013
C	-1.0615382568	-2.9559537884	0.7790902781
H	-0.5529371059	-3.7438092054	1.3526097499
C	-2.269005632	-3.5627428396	0.0475471239
H	-1.4248172007	-2.2229709044	1.5108062876
H	-2.8302779493	-2.7591458628	-0.4463072083
H	-2.9488818962	-3.9972839772	0.7913651768
C	-1.898749153	-4.6332399425	-0.9845986626

H	-1.3100008405	-5.4364172818	-0.5259397844
H	-1.3032370591	-4.2155036586	-1.8032320164
H	-2.7928736863	-5.0851547502	-1.4262892456
C	-2.4365833803	2.2280513648	-0.4891213283
H	-3.1177587059	0.2321741052	-0.8819756496
H	-2.0428915721	0.8535479821	-2.1151962874
H	-1.6156757069	2.8945193695	-0.7771114471
C	-2.6365234172	2.3057962727	1.0293005153
H	-3.3326368467	2.6276655772	-0.9830873758
C	-2.9930780794	3.7171424633	1.5049188914
H	-1.7234355114	1.9747864333	1.5396944106
H	-3.4255758873	1.6021297132	1.3285506741
H	-3.1242913955	3.7556169152	2.5911623087
H	-3.9233917211	4.0665286945	1.0427322191
H	-2.2054966368	4.4316507879	1.2385935582
C	2.6865229376	0.9600557178	0.8822742142
C	3.2824947713	2.3867677611	0.8802670702
H	2.497823833	3.1483191988	0.8487897198
H	3.8823736432	2.5575234631	1.7817868407
H	3.927086011	2.5363945721	0.0078502405
C	1.7925816646	0.7845790863	2.13195111
H	1.3616646356	-0.2213439799	2.1662522997
H	2.3792889863	0.933612281	3.0456225482
H	0.9675250501	1.502708603	2.1491336213
C	3.85014573	-0.0427997083	0.9859797866
H	4.4368105551	0.1633015936	1.8871657779
H	3.4925720776	-1.07540319	1.0542016822
H	4.5252022563	0.0305556584	0.1271245948
H	4.5252022563	0.0305556584	0.1271245948

TS exo 0458

E(RB3LYP) = -706.412095519 A.U.

First frequency = -490.5087 cm⁻¹

H	0.7270150786	-0.8643882397	-3.0774162587
C	0.6997126192	-0.1352433339	-2.2717665701
H	-0.0525954238	0.6357377008	-2.3961756904
C	1.8432518213	0.0801676434	-1.5197085141

C	1.8505721671	0.8995269801	-0.367916464
C	0.6931520353	1.5979587751	-0.0566345551
H	0.6281545503	2.1682246232	0.8635901639
H	0.0303564482	1.9427881725	-0.8394146871
C	-0.9690159636	-0.0308716796	0.1655152097
H	-0.6136268371	-0.1334173058	1.1877901448
C	-2.2064284708	0.8202480369	-0.0375525015
C	-0.6497676762	-1.041209918	-0.7376085336
H	-1.3560445801	-1.2210360393	-1.5465124581
C	0.1770214353	-2.2266129449	-0.2911065356
H	2.6820820978	-0.5842665624	-1.6951965707
H	1.0827047592	-1.8544832085	0.2029485816
H	0.5198854909	-2.7929308712	-1.1640192957
C	-0.5659101591	-3.1645801929	0.6830579897
H	0.100683177	-3.9983367414	0.9452743279
C	-1.892379021	-3.7271169354	0.1489211727
H	-0.7640655684	-2.6192646109	1.6146049045
H	-2.5916298839	-2.8981703896	-0.020027207
H	-2.3461019939	-4.3551329726	0.9261258397
C	-1.7494746793	-4.5433643636	-1.1401504904
H	-1.0325212575	-5.362718072	-1.0108504808
H	-1.3956814337	-3.9253168771	-1.9721341735
H	-2.7066975143	-4.9817340348	-1.4406912761
C	-2.4312863131	1.8980490113	1.0306701589
H	-3.0895057918	0.1622415627	-0.0500602896
H	-2.1731868437	1.2765333189	-1.037230898
H	-2.3737687797	1.4242232838	2.0199727364
C	-3.774692568	2.6317525525	0.9035472913
H	-1.6187721873	2.633407541	0.9960232227
C	-3.9130334799	3.4583885202	-0.3803215177
H	-3.8981652994	3.293662975	1.7700296489
H	-4.5934886637	1.9011733666	0.9588335036
H	-3.8936644397	2.8271609355	-1.2745162153
H	-3.0948182518	4.1827970798	-0.4693012855
H	-4.8550486982	4.0160837807	-0.3932117683
C	3.0195498575	0.8831001688	0.6410192732
C	4.178090203	-0.0266337893	0.1927818705
H	3.8679891846	-1.0740792888	0.1188474942

H	4.5824300576	0.2808640453	-0.7770962662
H	4.9925629577	0.0254482304	0.9226743467
C	3.5716456071	2.3190940353	0.7967567615
H	2.8007308628	3.0074326368	1.1552511626
H	4.401909421	2.3397731806	1.5123013313
H	3.9380130894	2.6996337292	-0.1624055847
C	2.5216327473	0.378812431	2.015245988
H	3.3414397142	0.3815079201	2.7427008725
H	1.7218544255	1.0074243939	2.4169478254
H	2.1380687913	-0.6439811456	1.9413395848
H	2.1380687913	-0.6439811456	1.9413395848

TS exo 0464

E(RB3LYP) = -706.413395606 A.U.

First frequency = -504.4008 cm^{-1}

H	0.2614156526	-1.1597199526	-2.902818151
C	0.3268694274	-0.3694948717	-2.1604695683
H	-0.2726675019	0.5032610743	-2.3922396041
C	1.4504025438	-0.2909433809	-1.3542475989
C	1.5537529182	0.62773802	-0.2856902196
C	0.5381674566	1.5645980577	-0.13604778
H	0.5362178118	2.237009488	0.7152811139
H	0.0271677893	1.9554314392	-1.0064462333
C	-1.4185538108	0.3642478998	0.0975576439
H	-1.1974989173	0.3722834961	1.1621385654
C	-2.435684589	1.3795872357	-0.3837683211
C	-1.2350738121	-0.8351334552	-0.5858451979
H	-1.9008932209	-1.0547314126	-1.4189419455
C	-0.6334696472	-2.0163344177	0.1389678346
H	2.1587941567	-1.1102121606	-1.4137548011
H	-1.26602435	-2.2603372331	1.0063273136
H	0.3335410397	-1.7061236053	0.5590214232
C	-0.4419182335	-3.2794018409	-0.7028341312
H	-1.4074901318	-3.5845971846	-1.1311576075
C	0.1527664601	-4.4448820181	0.0947354526
H	0.2126391106	-3.0558872446	-1.5536233885
H	-0.4991664851	-4.6725595094	0.9491241199

H	1.1148632741	-4.130877797	0.5231422175
C	0.3545240017	-5.7064835396	-0.749042554
H	0.7830550507	-6.5229440073	-0.1586942923
H	1.0294178643	-5.5129422111	-1.5907611803
H	-0.5967283746	-6.0583847189	-1.1645924476
C	-2.5526630437	2.6373437788	0.4840989235
H	-3.4241131141	0.8973652284	-0.4284896841
H	-2.2109690961	1.6691877178	-1.4220651547
H	-2.7489105401	2.338234863	1.5236678024
C	-3.6558548432	3.5920273201	0.0152552534
H	-1.5963917049	3.173653564	0.498160696
C	-3.7692413209	4.8467680113	0.8856331862
H	-4.6170671285	3.0602025314	0.0077720808
H	-3.4621541565	3.8828601494	-1.0263888782
H	-2.831312973	5.4138949311	0.8830412437
H	-3.9926067724	4.5850695735	1.9262819522
H	-4.5626962785	5.5127800205	0.5314453768
C	2.6498104993	0.5107545744	0.7953295704
C	3.5867068512	-0.689026556	0.5632830137
H	4.1001405538	-0.6230737896	-0.4013384172
H	4.3539788545	-0.7157921585	1.3439247299
H	3.0445066068	-1.6400006875	0.5988149842
C	3.504148553	1.7998968946	0.778073921
H	4.2936821747	1.7537888393	1.5373466019
H	3.9778193775	1.9381882156	-0.1994469942
H	2.8919430076	2.6840348929	0.9794665483
C	2.0094842963	0.3483485868	2.1931222205
H	1.357629031	1.1887005882	2.4476196688
H	1.4123446344	-0.5673064583	2.2476784821
H	2.7877461384	0.2913568295	2.962627265
H	2.7877461384	0.2913568295	2.962627265

TS exo 0469

E(RB3LYP) = -706.410708156 A.U.

First frequency = -524.5676 cm⁻¹

H	0.0721720632	-0.0000250822	-2.9743921397
C	0.3800258191	0.5660013447	-2.0990266832

H	-0.1038778817	1.5305788668	-2.0041621656
C	1.6377616685	0.3429448646	-1.5585372003
C	2.0524880872	0.9186450658	-0.3375029283
C	1.1703993176	1.786112133	0.2935018295
H	1.3838495764	2.1889916513	1.2763522798
H	0.5127820612	2.4094281755	-0.2995431599
C	-0.7173733877	0.5989786575	0.6685202672
H	-0.2020774247	0.089488692	1.4803840247
C	-1.6114309167	1.7393989873	1.1357883312
C	-0.9515636073	-0.1674686899	-0.4790504176
H	-1.805990655	0.0900748725	-1.0981959086
C	-0.5696352439	-1.6327860641	-0.48099972
H	2.2174519306	-0.4839901245	-1.961624945
H	0.4515135398	-1.7344404099	-0.0939590517
H	-0.5493697774	-2.0213409029	-1.5066351829
C	-1.5167790367	-2.4986506895	0.3671224739
H	-1.528156123	-2.1174118338	1.3972916887
C	-1.1309184063	-3.9820009179	0.3733055491
H	-2.545056178	-2.3890733072	-0.0062905695
H	-0.1011267062	-4.0836493292	0.7426667907
H	-1.1206292681	-4.357831702	-0.6589808042
C	-2.0700856229	-4.8416837429	1.2240861147
H	-2.0738568316	-4.5057862508	2.2674159312
H	-1.7732812131	-5.8956380441	1.2139475877
H	-3.1006523611	-4.7813846091	0.8557493305
C	-2.4651267853	2.4319893316	0.055078421
H	-1.0004977853	2.4901113286	1.6507754509
H	-2.2864060093	1.3432827777	1.9104397484
H	-2.6347202461	3.4771006078	0.3432518464
C	-3.8325287182	1.7727951197	-0.1808896271
H	-1.9093044059	2.4744987762	-0.8911852245
C	-4.6048026734	2.4053061777	-1.341134558
H	-4.4218688912	1.8501874504	0.7427313196
H	-3.7041907858	0.6993100967	-0.3624331543
H	-5.5873559499	1.9407881484	-1.4730739447
H	-4.0554133359	2.2978118758	-2.2836667751
H	-4.7618173634	3.4771122361	-1.1731456712
C	3.3299894732	0.3892966067	0.3452612451

C	3.6457735989	1.1396608232	1.6523256303
H	3.7520752887	2.215842754	1.4822976495
H	2.8666465792	0.987985914	2.4065653462
H	4.586309063	0.7713266538	2.0751402172
C	3.1811581564	-1.1130658102	0.681926365
H	2.3479836812	-1.2745795189	1.3740748787
H	2.994562034	-1.7130872336	-0.2131653738
H	4.0931228748	-1.4943812407	1.1559949677
C	4.5250383411	0.5801397556	-0.6165433711
H	5.4489280943	0.2108591192	-0.156695968
H	4.3820498996	0.0391098677	-1.5562821106
H	4.6629597021	1.6388273279	-0.8588863868
H	4.6629597021	1.6388273279	-0.8588863868

TS exo 0473

E(RB3LYP) = -706.411691220 A.U.

First frequency = -505.9293 cm⁻¹

H	0.600128226	0.2164717336	-3.29168199
C	0.6215731634	0.6541054134	-2.2971285708
H	-0.1097254625	1.4362329371	-2.1393713424
C	1.7903846528	0.5898794882	-1.5558963536
C	1.8557335695	0.992835848	-0.2039725407
C	0.711174212	1.5397700978	0.3629667586
H	0.6759008582	1.770647999	1.4233493083
H	0.0367893069	2.1366035373	-0.2368903159
C	-0.8811804559	-0.064310305	0.1774194759
H	-0.3984889135	-0.5523684287	1.0193433741
C	-2.096215191	0.7646635583	0.5601422644
C	-0.7288342894	-0.6839039895	-1.0640909513
H	-1.5049434078	-0.5325653583	-1.810926652
C	0.0359146891	-1.9854575318	-1.1839154048
H	2.6022281166	-0.0021147712	-1.9642731333
H	0.9124241855	-1.9441790595	-0.5241508695
H	0.4260970565	-2.098944847	-2.2015287066
C	-0.7983428772	-3.2392270217	-0.8453628247
H	-1.6752229002	-3.2774646014	-1.5075565203
C	-1.2652644849	-3.3434562045	0.6108840358

H	-0.1977939501	-4.1273019655	-1.0884855144
H	-1.9198601988	-2.4970245613	0.8479164927
H	-0.3953771199	-3.250819021	1.2762598256
C	-1.9995996591	-4.6555713368	0.9020564726
H	-1.3554590967	-5.5214895518	0.7102654737
H	-2.8864660138	-4.7589365526	0.2660568173
H	-2.3297704561	-4.7097206953	1.9446939744
C	-2.7544752793	1.5671259044	-0.570696159
H	-1.8226589073	1.442549452	1.3767535312
H	-2.8548307066	0.0880072116	0.9857169264
H	-2.0147456868	2.2306605265	-1.0386688494
C	-3.9564384275	2.4091053697	-0.113186607
H	-3.0871162796	0.8794058651	-1.3571809312
C	-3.5922634158	3.5676002043	0.8227829051
H	-4.6887418803	1.7544459884	0.3790689429
H	-4.4589616652	2.8141245169	-1.0005511589
H	-4.4726256135	4.1720716896	1.0639575289
H	-2.8513795095	4.2279161108	0.3568722013
H	-3.1698804857	3.2130509837	1.7681689058
C	3.0535855923	0.6331532484	0.70016421
C	4.1981044675	-0.0459458022	-0.0742591689
H	5.0402686139	-0.2335913594	0.5998299883
H	3.8911667333	-1.0096399924	-0.4933214154
H	4.5613816376	0.5839949234	-0.8927714866
C	3.6111403951	1.9256706585	1.3399961192
H	3.9510757467	2.6244140708	0.5684953858
H	2.8520862105	2.4359723974	1.9400082848
H	4.4610886643	1.6986551388	1.994076763
C	2.5952462529	-0.3308341563	1.8188878711
H	1.8095247573	0.1083962214	2.4403906359
H	2.2062030123	-1.2630167802	1.3962020683
H	3.4357660207	-0.5815695994	2.4761567633
H	3.4357660207	-0.5815695994	2.4761567633

TS exo 0474

E(RB3LYP) = -706.411641186 A.U.

First frequency = -504.3495 cm^{-1}

H	0.6695411499	0.2549422255	-3.2849071139
C	0.7354684096	0.6984738632	-2.2949854158
H	0.062176241	1.5303603478	-2.1341070377
C	1.905939999	0.5583034183	-1.5676799093
C	2.017165145	0.966721357	-0.2202417581
C	0.9197774985	1.5934824628	0.3572865364
H	0.9154173178	1.8351980898	1.4158220653
H	0.2783510451	2.229273565	-0.2389613651
C	-0.7760675233	0.1002829291	0.213346945
H	-0.3114089414	-0.4180732192	1.047338916
C	-1.9296027655	1.0042795993	0.6156449365
C	-0.6922739354	-0.5322495488	-1.0282734896
H	-1.4691900594	-0.3262400731	-1.7610322489
C	-0.0261561466	-1.8861013073	-1.1567463739
H	2.6696791079	-0.0913575005	-1.9811862155
H	0.8617967511	-1.9072151785	-0.5114806414
H	0.3375564731	-2.0304939232	-2.1802108731
C	-0.9441550925	-3.0746489168	-0.7997737511
H	-1.8316129905	-3.0509676517	-1.4484163045
C	-1.3950268846	-3.1392506578	0.6637770236
H	-0.4138674641	-4.0050698503	-1.0478922586
H	-1.9814199683	-2.2457989959	0.9067710415
H	-0.5106270276	-3.1091433674	1.315628153
C	-2.2200753386	-4.3922885965	0.9717855077
H	-3.1219346782	-4.431509298	0.3498507858
H	-2.5370914136	-4.4184888726	2.0195707889
H	-1.6449925302	-5.3042306424	0.7739161159
C	-2.5679141811	1.8283124576	-0.5111689527
H	-1.6016024794	1.6895903264	1.4087870635
H	-2.7025143461	0.3730897498	1.0783923927
H	-1.7866314002	2.3859753108	-1.0425919791
C	-3.6351436181	2.8206723466	-0.0233828093
H	-3.0200067868	1.1564056305	-1.2522733961
C	-4.8662814282	2.158338827	0.605956732
H	-3.955918999	3.4366821353	-0.8729689216
H	-3.1808824463	3.5116809453	0.6999287247
H	-4.6122186304	1.6106656528	1.5189658313
H	-5.3265044805	1.4466707026	-0.0895815471

H	-5.623667152	2.9033661801	0.8703273716
C	3.1999205531	0.5326562285	0.6710957185
C	4.2898817573	-0.2187841578	-0.1152624868
H	5.1272377529	-0.4568411719	0.5488256735
H	3.9183034396	-1.1626435906	-0.5269927998
H	4.6811341642	0.3850464762	-0.9405557438
C	3.8466660066	1.7873226507	1.3022049173
H	4.2217043241	2.4620502242	0.5256176223
H	3.1293765372	2.3459929845	1.9103963372
H	4.6879192869	1.5067084411	1.9466338972
C	2.6934326885	-0.3989383803	1.7964552045
H	3.5235097899	-0.7031624884	2.4443721432
H	1.944966281	0.0907519407	2.4261946984
H	2.2399310008	-1.3042384862	1.3795794376
H	2.2399310008	-1.3042384862	1.3795794376

TS exo 0475

E(RB3LYP) = -706.412501539 A.U.

First frequency = -492.7790 cm⁻¹

H	0.884910627	-1.57705159	-2.6604613009
C	1.0012730643	-0.6326742571	-2.1366051496
H	0.4800960949	0.1992400228	-2.5946544692
C	2.0929489971	-0.4481365535	-1.3075210412
C	2.244146088	0.6905439667	-0.4831059198
C	1.3022170055	1.7072083939	-0.6094694887
H	1.3273220013	2.5665684233	0.0539190843
H	0.8685197148	1.9184777412	-1.5786740125
C	-0.6904263837	0.8000944936	-0.1338570115
H	-0.4775127111	0.98797624	0.9151867367
C	-1.5875568417	1.8087616861	-0.8232103472
C	-0.6828821706	-0.5298199445	-0.5467752623
H	-1.3336850341	-0.8126101815	-1.3689399698
C	-0.2585139259	-1.618433653	0.4141551346
H	2.7295198618	-1.3087332506	-1.131862603
H	-0.7778444411	-1.4793841486	1.3746393722
H	0.8063657984	-1.4708357899	0.6398180429
C	-0.4969711405	-3.0566968487	-0.07802836

H	-0.2958511356	-3.105847764	-1.1562398658
C	-1.9040642034	-3.6075625768	0.2122964473
H	0.2318637262	-3.7248351806	0.3968926317
H	-2.0481764401	-3.645859592	1.3009230478
H	-1.9517824381	-4.6474088183	-0.1363498122
C	-3.0572625414	-2.8155335684	-0.4142847336
H	-4.0201192331	-3.2942114786	-0.2069557062
H	-2.9467479097	-2.7478904106	-1.5029800984
H	-3.1034996467	-1.7944405674	-0.0227075706
C	-3.0860169577	1.5989580945	-0.5259375718
H	-1.4370688431	1.7446349765	-1.9099414908
H	-1.3007979471	2.8271462282	-0.5319435766
H	-3.6696022804	2.3392559667	-1.0909472414
C	-3.4499285623	1.6982990162	0.959580659
H	-3.3885290913	0.6127843086	-0.9032191034
C	-4.9472317648	1.5053762177	1.2151809499
H	-3.129018274	2.6753035043	1.3471356486
H	-2.8838875811	0.9452735442	1.522028445
H	-5.1873152655	1.5779808123	2.2809746478
H	-5.2803087517	0.5217007863	0.8643592088
H	-5.5397897856	2.2611096648	0.6868008212
C	3.2746102841	0.7444307639	0.6640004568
C	2.5447745336	0.8849439443	2.0199065764
H	3.2700688412	0.9407499007	2.8397157973
H	1.930057289	1.7887202078	2.0623292814
H	1.8909296502	0.0261702012	2.2021500387
C	4.157910643	-0.5149550818	0.7281982275
H	4.8920959918	-0.4110257529	1.5337761334
H	3.5689982065	-1.4151109012	0.9328924108
H	4.7096018531	-0.6706921802	-0.2045589287
C	4.1982812822	1.9671109488	0.4553944557
H	4.9387984554	2.0357552468	1.2608417604
H	4.7348225355	1.8899611099	-0.4960245441
H	3.628352189	2.9007767382	0.4414708236
H	3.628352189	2.9007767382	0.4414708236

TS exo 0476

E(RB3LYP) = -706.412502972 A.U.

First frequency = $-510.8199 \text{ cm}^{-1}$

H	0.4689590086	-1.1111945544	-2.8878688619
C	0.6851800305	-0.2778993214	-2.2260203308
H	0.4206943412	0.6891034434	-2.638834836
C	1.6925988002	-0.40537543	-1.2826264905
C	1.9577530766	0.5871389008	-0.3119137607
C	1.2321912945	1.7694826576	-0.3891558127
H	1.3169897358	2.5344256591	0.3734844115
H	0.9369106692	2.151298219	-1.3578019871
C	-0.9652844129	1.1775124601	-0.28357583
H	-0.8396585097	1.1703591191	0.7947949423
C	-1.5640639156	2.4308725383	-0.8843448787
C	-1.1162530899	-0.0590067859	-0.9138811893
H	-1.7221310479	-0.0898842643	-1.8189148701
C	-1.0863476814	-1.3190725359	-0.0785649647
H	2.1326784952	-1.390922502	-1.1490891998
H	-1.9244905283	-1.282524112	0.6358174182
H	-0.1765482885	-1.2987520174	0.5308532668
C	-1.1740132057	-2.6353892352	-0.8568158352
H	-2.0488425607	-2.598843063	-1.5204522338
C	-1.272131742	-3.8791045169	0.0394482885
H	-0.2977298676	-2.7354588418	-1.5082264118
H	-1.4462370452	-4.7586245923	-0.593357417
H	-2.153857431	-3.7914347975	0.689120851
C	-0.0259935525	-4.1212101733	0.8998470987
H	0.8722784656	-4.1914647324	0.274592794
H	-0.1099590062	-5.0533490252	1.4680153763
H	0.136783397	-3.3113674692	1.6175799092
C	-3.1054507027	2.5239895487	-0.8345547031
H	-1.2631336595	2.4939678415	-1.9404341257
H	-1.1423699701	3.3179610127	-0.3947989759
H	-3.3959717077	3.4140247579	-1.4085783213
C	-3.7357055635	2.622438473	0.5666484454
H	-3.5351681859	1.6633917108	-1.3646603961
C	-3.8587508754	1.2955228187	1.3270754148
H	-4.7414132857	3.0489541096	0.4598245673
H	-3.1670084725	3.3447122171	1.1688930216

H	-4.4032733437	1.4327310341	2.2675610736
H	-2.8845388649	0.8635154242	1.5661542054
H	-4.4049416552	0.5558895091	0.7302541001
C	2.8916199632	0.2537168155	0.8700212045
C	4.2870869222	-0.0999051138	0.3045245368
H	4.2470065542	-0.9671670751	-0.3608688801
H	4.6989402936	0.7391522874	-0.2654071575
H	4.9820084764	-0.3353079126	1.1189003713
C	3.0546252558	1.4411181778	1.8364047578
H	3.7543987227	1.1767060023	2.6360423212
H	3.4481110142	2.3255946724	1.3254541045
H	2.1045330867	1.712931219	2.308274451
C	2.3557368984	-0.9486168766	1.6812544201
H	1.3844736961	-0.7127338855	2.1286489792
H	2.2312454061	-1.8389467679	1.0591463249
H	3.0467866423	-1.2031088936	2.4932433338
H	3.0467866423	-1.2031088936	2.4932433338

TS exo 0477

E(RB3LYP) = -706.413219706 A.U.

First frequency = -504.0773 cm^{-1}

H	1.3606092554	-0.5919084479	-3.3137350585
C	1.207470138	0.1182208694	-2.5051643604
H	0.7474639322	1.0496718641	-2.8165636118
C	2.0368672507	0.0642599099	-1.395326067
C	1.8155448359	0.8512620616	-0.2416703347
C	0.7862519059	1.7789848721	-0.2778822684
H	0.5174941917	2.3523878532	0.5992978438
H	0.5147829381	2.2496121225	-1.2139838826
C	-1.1223984378	0.5391147775	-0.7471214304
H	-1.1318040414	0.2679823085	0.3041075288
C	-2.0724747984	1.6413688065	-1.1712976703
C	-0.7463404281	-0.4567959053	-1.6496933737
H	-1.178120599	-0.4027972647	-2.6491532318
C	-0.4265157573	-1.8445680389	-1.1391110609
H	2.7256851619	-0.7738923224	-1.3241102259
H	0.2777303301	-1.7473370833	-0.307469729

H	0.0885284704	-2.4292723839	-1.9118208691
C	-1.6741820669	-2.6155937802	-0.6714349436
H	-2.1826393939	-2.033359125	0.1095615346
C	-1.3705938903	-4.0247584717	-0.1391763091
H	-2.3835202142	-2.6870539015	-1.5067961904
H	-0.8581230013	-4.6040922301	-0.919629983
H	-2.3187960105	-4.5435260259	0.0515863953
C	-0.5281578959	-4.0357286911	1.1423671017
H	-0.3942786707	-5.0544289776	1.5207434575
H	-1.0111528442	-3.4475542159	1.9318411223
H	0.4677376845	-3.6116880781	0.9801994843
C	-2.2815334273	2.8009382245	-0.1798670385
H	-3.051260547	1.1826617281	-1.374608582
H	-1.7438015662	2.0509823646	-2.137139124
H	-1.392106841	3.4396700261	-0.1577096649
C	-2.6233123351	2.3756527374	1.2576980331
H	-3.0956840757	3.4296666146	-0.5647474946
C	-3.8475436477	1.4597481094	1.3633535925
H	-2.7926748828	3.2799403307	1.8556812782
H	-1.7559441267	1.8780200781	1.7100871109
H	-4.095061418	1.2481976862	2.4085672943
H	-3.675318311	0.500344839	0.8644505787
H	-4.7266474873	1.9213234422	0.8986029369
C	2.5824259405	0.5150433283	1.0543600618
C	2.2743289435	-0.9293396968	1.5140373714
H	2.5403075729	-1.6651243379	0.7497521954
H	2.8386943327	-1.1728548601	2.4216291898
H	1.2092134056	-1.047911388	1.7385159429
C	4.0982046182	0.6494939764	0.781395912
H	4.4311047844	-0.0312892001	-0.0073454968
H	4.3471311788	1.6688607947	0.4692269892
H	4.6723054012	0.4182741513	1.6860434686
C	2.218967922	1.4650472485	2.2104224088
H	1.1637667711	1.3783823726	2.4904285774
H	2.8142466661	1.2183424885	3.0957137955
H	2.419364884	2.5096500728	1.9518680427
H	2.419364884	2.5096500728	1.9518680427

TS exo 0484

E(RB3LYP) = -706.412528505 A.U.

First frequency = -511.2691 cm⁻¹

H	0.1947396538	-1.4843261931	-2.4790666867
C	0.5056545303	-0.5764982584	-1.9713942009
H	0.0998196854	0.333348331	-2.3959183336
C	1.6829535849	-0.5834333371	-1.2415688989
C	2.0878552527	0.5034795611	-0.4372606495
C	1.3209548915	1.6639135788	-0.4967713947
H	1.5339869836	2.500361423	0.1623766991
H	0.8693787973	1.9549363514	-1.4370376163
C	-0.7455179656	1.1144817989	0.1230960597
H	-0.4420639529	1.2766939085	1.155577252
C	-1.5132190138	2.260425464	-0.5037712696
C	-0.9911691322	-0.2072457698	-0.2567131533
H	-1.7540398277	-0.3781539711	-1.0121379964
C	-0.7304962661	-1.3372297196	0.7205511507
H	2.185455936	-1.5372690985	-1.1222405102
H	-0.8678145256	-0.9577974688	1.7419038335
H	0.3233140609	-1.6426889738	0.6698738239
C	-1.6534138404	-2.5550902596	0.5386977087
H	-1.5031678508	-3.2383896421	1.3855622242
C	-1.4691939395	-3.34566916	-0.766240158
H	-2.6950242104	-2.2123164437	0.6037718259
H	-1.617877975	-2.6809899434	-1.6257174256
H	-2.2627711193	-4.1011818497	-0.8298136096
C	-0.1086031884	-4.0403039674	-0.8810155331
H	0.7133604668	-3.3190236344	-0.8693261962
H	-0.0319009269	-4.6149364673	-1.8099232196
H	0.0484157862	-4.7329289689	-0.0459481035
C	-2.8511384586	2.565291015	0.2032756514
H	-1.7076505934	2.0324643471	-1.5616117362
H	-0.9092511577	3.1758847322	-0.4919050798
H	-2.6513231345	2.7986087641	1.2588289157
C	-3.89706506	1.4480169529	0.1250104072
H	-3.2737634038	3.4802895989	-0.2347425239
C	-5.2222610424	1.8328272358	0.789136891

H	-3.4991627267	0.5413884905	0.595130274
H	-4.0722519524	1.1912399705	-0.9291737051
H	-5.9543630562	1.0211592948	0.7254262007
H	-5.6622227638	2.7174885165	0.3144793136
H	-5.0766279815	2.0673648665	1.849976961
C	3.1763112517	0.3613347151	0.6459115777
C	3.8697366696	-1.0129717828	0.6125316898
H	3.1714009085	-1.8274887684	0.8306455983
H	4.332281206	-1.2088716876	-0.3603975133
H	4.6606007402	-1.0464015386	1.3689286051
C	4.2562766115	1.4469207672	0.4333962223
H	5.0363067805	1.372040309	1.1999375059
H	4.7299830948	1.3360285789	-0.5476113135
H	3.8302542424	2.4530701064	0.4855579623
C	2.5377971745	0.5418664348	2.0426450071
H	3.2983597388	0.4495915832	2.8265093114
H	2.0681014723	1.5238817778	2.1519199449
H	1.7704481282	-0.2184488886	2.2199653255
H	1.7704481282	-0.2184488886	2.2199653255

TS exo 0486

E(RB3LYP) = -706.411494294 A.U.

First frequency = -497.2331 cm^{-1}

H	0.7312975364	-0.550600491	-3.2612448928
C	0.7455072223	0.1130147956	-2.4003767631
H	0.1615027886	1.0177364969	-2.5293570818
C	1.8248242917	0.0625548502	-1.5315724102
C	1.8545714259	0.7844746158	-0.3173100486
C	0.8135110551	1.6632346186	-0.0551299766
H	0.7536090524	2.1708375994	0.9015229422
H	0.3115562639	2.1794234176	-0.8627799343
C	-1.1311904543	0.3599646108	-0.1479186733
H	-0.9176789536	0.1368107657	0.894333181
C	-2.1654007922	1.4363080579	-0.4107144733
C	-0.8868245133	-0.6372479874	-1.0888156737
H	-1.5247754068	-0.6535224673	-1.9717027505
C	-0.3205779274	-1.9691237264	-0.6513167989

H	2.5461835896	-0.7321107384	-1.6863939022
H	0.5476018383	-1.7850621596	-0.0047153404
H	0.0568479568	-2.5160454603	-1.5217697607
C	-1.3364269048	-2.8365511937	0.1144586242
H	-1.7372036172	-2.2503384844	0.9508030134
C	-0.7517291164	-4.1513248116	0.6536736714
H	-2.1920079245	-3.0577718498	-0.5394086506
H	-1.5059501918	-4.641027707	1.2829595511
H	0.0948883171	-3.9214819403	1.3157441141
C	-0.2968412828	-5.1308832672	-0.4343356922
H	0.047546777	-6.0746956543	0.0009832043
H	0.5271766102	-4.7242224472	-1.0291567088
H	-1.1190550591	-5.3610231053	-1.1221583838
C	-2.3637749968	2.4228646162	0.7464628533
H	-3.1241892353	0.9491512077	-0.635458634
H	-1.9033517819	1.9925765565	-1.3246736118
H	-2.6457770281	1.8600795164	1.6479751374
C	-3.41700777	3.5083897518	0.4768294195
H	-1.408311814	2.9068248987	0.9763932784
C	-4.8466644779	2.9769662953	0.320519443
H	-3.1333340403	4.0682863677	-0.4251212743
H	-3.3943186553	4.2315054201	1.3019498281
H	-4.9463888261	2.3230794475	-0.5516150891
H	-5.561839157	3.7969282589	0.1983787188
H	-5.1479761939	2.3997958185	1.2025785753
C	2.8885028002	0.4820487384	0.7894417217
C	3.8987127032	-0.6045336404	0.3774479751
H	4.6259770606	-0.7571181748	1.181592845
H	3.4082641447	-1.5652106298	0.189172119
H	4.4546346995	-0.3208421998	-0.5220682783
C	3.6769400518	1.7734929251	1.1081521521
H	4.204935376	2.1345343788	0.219386002
H	3.0127617648	2.5733640598	1.4484452205
H	4.417737262	1.5915371041	1.8955110122
C	2.1669999286	-0.0003908969	2.0691066068
H	2.8939200641	-0.1963200293	2.8656338673
H	1.4579707431	0.7425410631	2.4451118886
H	1.6135799899	-0.9262327797	1.8814148775

H 1.6135799899 -0.9262327797 1.8814148775

TS exo 0489

E(RB3LYP) = -706.413635520 A.U.

First frequency = -481.3212 cm⁻¹

H 0.8388776921 -1.7165143534 -2.5655284169
C 0.8988154988 -0.7488650959 -2.0764547472
H 0.3620679867 0.0419612001 -2.5859013014
C 1.9479064455 -0.4853617155 -1.2150702551
C 2.0259691921 0.6973132917 -0.4431500293
C 1.0504495003 1.66532038 -0.6474772997
H 1.0123553047 2.5529343652 -0.0232136669
H 0.6236942247 1.8057875277 -1.6321884071
C -0.9241340826 0.6653720499 -0.1760944907
H -0.7203411338 0.8876128462 0.8683422755
C -1.8531971502 1.6232612425 -0.8898424192
C -0.8469812744 -0.6694672721 -0.562444414
H -1.4780860109 -0.9903057738 -1.3873469658
C -0.4217030077 -1.7142748078 0.4432490642
H 2.6063786513 -1.3128182062 -0.9730769523
H -1.1561486325 -1.7257086041 1.2619168583
H 0.5193679056 -1.382926156 0.9027113127
C -0.241884155 -3.1458624471 -0.0841134776
H 0.6436171472 -3.185853232 -0.7284046129
C -1.444686252 -3.7159275535 -0.8542036622
H -0.0288414197 -3.7994139703 0.7725003619
H -1.2209821071 -4.7545021805 -1.1289959977
H -1.5642257526 -3.1776108935 -1.8031858544
C -2.7632745033 -3.6681144462 -0.0746760073
H -3.5706722814 -4.1558767068 -0.6303858013
H -3.0742913759 -2.6368459513 0.1225624648
H -2.6686317735 -4.17591532 0.8923281324
C -3.3371873986 1.4263952388 -0.5109228683
H -1.7521789508 1.4868295046 -1.9753829129
H -1.5588074228 2.6591163156 -0.6856980554
H -3.9393773612 2.1740197892 -1.0460637526
C -3.6338957223 1.5213767385 0.9940077638

H	-3.6629826392	0.4429589256	-0.8732269212
C	-3.2232681286	2.8548058125	1.6277647842
H	-3.1263952503	0.6990758117	1.5139520363
H	-4.7084422228	1.362041219	1.1487566685
H	-2.1386430338	3.0022122224	1.590233162
H	-3.5245313141	2.9035801273	2.6791493289
H	-3.6888383919	3.6997981125	1.106926039
C	3.0183265629	0.850463194	0.7287220375
C	2.2473801935	1.0501590551	2.0540248484
H	1.6023474213	1.9330046211	2.0247798586
H	1.617594162	0.1825963903	2.2755459763
H	2.9481890754	1.1816587623	2.8863413754
C	3.9353320786	-0.3753060871	0.8937587891
H	4.6382936755	-0.2035088525	1.7154189667
H	3.3658400814	-1.2802566579	1.129938741
H	4.5232229259	-0.5661432026	-0.0099076563
C	3.9110027505	2.0867766868	0.4711775865
H	3.3132765684	2.9990228138	0.3852615702
H	4.6261042763	2.2269288136	1.2902486329
H	4.4761509936	1.9698570627	-0.4593767857
H	4.4761509936	1.9698570627	-0.4593767857

TS exo 0494

E(RB3LYP) = -706.411398616 A.U.

First frequency = -516.0469 cm^{-1}

H	1.3578949853	-0.6096963416	-3.2615693917
C	1.247210889	0.128723117	-2.4712639788
H	0.7813644732	1.0531599659	-2.7977398392
C	2.1518546851	0.1205543704	-1.4168245845
C	2.0063596514	0.9539054729	-0.2849153266
C	0.9744649749	1.8800513409	-0.2924855577
H	0.7588907048	2.4899862759	0.5753358287
H	0.646815851	2.3136178344	-1.22747173
C	-0.9711732036	0.625815099	-0.6445655612
H	-0.9312603248	0.4277328756	0.4211585901
C	-1.8888849106	1.746144445	-1.099609423
C	-0.6229594804	-0.4147046025	-1.5088974251

H	-1.1124143836	-0.4199514697	-2.4831832276
C	-0.2820824762	-1.7777855286	-0.9450844876
H	2.8458086832	-0.714233475	-1.3580136757
H	0.4500376932	-1.6525824655	-0.1391993199
H	0.2067527173	-2.3933678486	-1.7105297487
C	-1.5065969919	-2.5291523692	-0.396706088
H	-1.9793204791	-1.9228072503	0.387601149
C	-1.1594328478	-3.9109990149	0.1683267268
H	-2.2588833052	-2.6362453605	-1.1910994361
H	-0.4007216305	-3.7970654953	0.9548317342
H	-0.6908231612	-4.5173423977	-0.6188696477
C	-2.3770131799	-4.6497462982	0.7310429498
H	-3.1371250712	-4.8028611433	-0.0436571744
H	-2.844043173	-4.077848947	1.5411054742
H	-2.1046255676	-5.6323548274	1.1300985
C	-2.3517638984	2.7078015717	0.0127212978
H	-2.778829955	1.3141163632	-1.5814087649
H	-1.3902076152	2.3194706296	-1.894910208
H	-1.5304786098	2.8645344288	0.7234402287
C	-3.6074089619	2.2513899936	0.7753717725
H	-2.5631830727	3.6895497856	-0.4280572347
C	-3.4713542294	0.9164301034	1.5158167862
H	-4.4448477801	2.1845348642	0.0671689197
H	-3.8808691211	3.0343515668	1.4946006254
H	-3.2978369867	0.0881068981	0.8223287295
H	-4.3792555033	0.6887227047	2.084134184
H	-2.6328822399	0.9386113332	2.2218890128
C	2.8624476232	0.6740510477	0.9679416712
C	2.5830091611	-0.7452821203	1.5142820922
H	1.5355506626	-0.8445023825	1.8180585687
H	2.7911192854	-1.5171089598	0.7680311865
H	3.2090042795	-0.950378437	2.3904787297
C	4.3556965384	0.7865844591	0.5833344915
H	4.9909754463	0.5959994123	1.4559972161
H	4.6315895391	0.0667315882	-0.1925931406
H	4.5846702042	1.7883251695	0.2056831823
C	2.584373706	1.6797286112	2.1002812922
H	1.5519857973	1.6115271605	2.4589740158

H	3.2414225971	1.4727010163	2.9514278075
H	2.7670984224	2.7097563272	1.7779396751
H	2.7670984224	2.7097563272	1.7779396751

6 Regioselective intramolecular radical H-atom transfer

6.1 1,5 HAT

6.1.1 Starting TS

TS input

E(UwB97XD) = -1036.74514643 A.U.

First frequency = -1538.7560 cm⁻¹

S	0.9343104449	-1.3529772657	-0.1521547035
O	1.9684543252	-1.7138327534	-1.1339189767
O	0.0389090473	-2.4259617742	0.2965485901
N	-0.0307981594	-0.1070857636	-0.7003235969
C	0.72749986	1.0574240578	-1.1914861117
H	1.454561802	0.7515289906	-1.9554373412
H	0.0053987766	1.7242396604	-1.6745360804
C	1.4137783813	1.7835877088	-0.0413199043
H	1.7484081653	0.7598497272	0.6779196861
C	-1.2417156122	-0.4624889356	-1.4568553704
H	-1.4546485867	-1.518959162	-1.2865840325
H	-1.0571376843	-0.3335725631	-2.5307251585
C	-2.4230671652	0.3957463747	-1.0067352732
H	-3.2696770548	0.1884194323	-1.6749564185
H	-2.1714688664	1.4548172118	-1.1509236004
C	-2.8520832526	0.1726390808	0.4496661509
H	-1.9498998137	0.2370230192	1.0726355205
C	-3.8169576715	1.2747517892	0.8929736769
H	-3.357561135	2.2651141248	0.8008250747
H	-4.1193715237	1.1378211706	1.9364120357
H	-4.7248895711	1.2664176993	0.2771418443
C	-3.4728664384	-1.2112666551	0.6598182502

H	-3.7734128179	-1.345498993	1.7041902448
H	-2.7712657678	-2.0137842456	0.4139703624
H	-4.3665803681	-1.3321139608	0.0348871127
C	1.7237375887	-0.5357821569	1.2021975957
H	1.0136976572	-0.4508008628	2.0248207033
C	3.1202682911	-0.9811639549	1.539579885
H	3.5293281445	-0.318402176	2.3064084284
H	3.7679530588	-0.9431984981	0.660937492
H	3.1369479413	-2.0031579287	1.9355960607
C	0.4609998407	2.5652361501	0.8377400833
H	0.1002368214	3.4553136936	0.3044397143
H	-0.4088846158	1.959157756	1.1087869622
H	0.9523219826	2.9005431016	1.7559633845
C	2.6864969432	2.5036173755	-0.4224610242
H	2.467785854	3.3305620689	-1.1123542238
H	3.1751522476	2.9291087031	0.4588401989
H	3.3915219307	1.8310997529	-0.9210892414
H	3.3915219307	1.8310997529	-0.9210892414

6.1.2 Lowest TS

TS 6-311++G(d,p) 0003

E(UwB97XD) = -1036.89360521 A.U.

First frequency = -1540.9853 cm⁻¹

S	0.5199260131	-1.1670637656	1.1452609419
O	-0.5527158201	-2.1547267214	1.0585061347
O	1.2088328916	-1.0360186322	2.4307392974
N	-0.1178296063	0.2926458702	0.6393320145
C	0.844892798	1.4048532652	0.722515162
H	0.2890731529	2.320295203	0.5007798609
H	1.2367062878	1.4967512409	1.742647947
C	1.9757455512	1.2355410476	-0.2825600688
H	2.1040590209	-0.0547740592	-0.2524703062
C	-1.4909649627	0.6081262046	1.0613251161
H	-1.4692648925	1.2434662579	1.954676922
H	-1.9847756909	-0.3229434417	1.3372776147
C	-2.2641425239	1.297437571	-0.0597808422

H	-1.7890322727	2.2569450227	-0.2963620475
H	-3.2618897701	1.5397169135	0.3272070195
C	-2.4029275936	0.4788606388	-1.3479379479
H	-1.3920634312	0.2356438927	-1.6940245631
C	-3.1482459037	-0.8372913841	-1.1223852696
H	-4.1463145025	-0.6499382884	-0.709434428
H	-2.6105884045	-1.4954469541	-0.4358187383
H	-3.2733906214	-1.3745671046	-2.0669969493
C	-3.0841808536	1.316515251	-2.4300080559
H	-2.5339657992	2.2429897797	-2.620753794
H	-4.1020782023	1.5867731902	-2.1270967666
H	-3.1517033795	0.7636114447	-3.3712226093
C	1.7492644616	-1.4011178353	-0.0964747511
H	2.6154596267	-1.8903471487	0.3430097336
C	1.2587762494	-1.9038470294	-1.4252479349
H	0.9656463896	-2.9562467986	-1.3693745525
H	2.0556632714	-1.8117387829	-2.1663581716
H	0.3980533065	-1.327998642	-1.7714074422
C	3.2970240219	1.8157957759	0.1610032094
H	3.2238737703	2.9074243351	0.2514598066
H	3.5992880064	1.4206058001	1.1343595017
H	4.0848244854	1.5971312471	-0.5639134733
C	1.5772118413	1.5547409948	-1.7056507063
H	1.4679211703	2.6399182609	-1.8280725452
H	2.332271827	1.2130054543	-2.4180261285
H	0.6215628357	1.0925309631	-1.9624136004
H	0.6215628357	1.0925309631	-1.9624136004

6.1.3 Additional TS

TS 6-31++G(d,p) 0001

E(UwB97XD) = -1036.74434301 A.U.

First frequency = -1545.2213 cm⁻¹

S	0.2674546397	-1.2281210715	0.2942976529
O	-0.378211832	-2.3027469373	-0.4672269417
O	-0.1805610379	-1.0061743203	1.6768151058
N	0.1459383387	0.1576030759	-0.6241249638

C	0.723051455	1.3559076244	0.0053089982
H	0.4953537703	2.1978114093	-0.6578480161
H	0.2459438862	1.5598231378	0.9723443156
C	2.2365414054	1.228486964	0.1596700459
H	2.3356619114	-0.0458425295	0.3921326985
C	-0.9904181183	0.3395782494	-1.5398999726
H	-1.3128045362	-0.6527961762	-1.8589481291
H	-0.5873637552	0.8445423001	-2.4250810868
C	-2.1640387287	1.1565763707	-0.9931289378
H	-2.877427413	1.2800123989	-1.8200716425
H	-1.8129978775	2.1667628792	-0.746639615
C	-2.8999359119	0.5743574492	0.220113852
H	-2.1626365372	0.3911243513	1.0121659025
C	-3.915392893	1.5908531896	0.7496042874
H	-3.4292100313	2.5326533347	1.0264938535
H	-4.4325441791	1.2049598376	1.6342034185
H	-4.673625824	1.8141498216	-0.0114092384
C	-3.5878368761	-0.7543833415	-0.1061493447
H	-4.1201691878	-1.1381664078	0.7704168329
H	-2.8729294461	-1.520875587	-0.4184288893
H	-4.3205610477	-0.6193057645	-0.9119934378
C	2.0233449242	-1.4075141805	0.3530409293
H	2.3144691071	-1.8155066058	1.320071793
C	2.6742605275	-1.9922534176	-0.8708635836
H	2.3158154112	-1.5053897373	-1.7815536727
H	2.4739256742	-3.0655750596	-0.9539050111
H	3.7566414759	-1.8514036594	-0.8084901732
C	2.8066397096	1.9423700354	1.3635954825
H	2.3108676607	1.6261016327	2.2865155178
H	3.8794120352	1.7518343547	1.460946021
H	2.6701793622	3.0282779431	1.2646494839
C	2.994712426	1.4383996861	-1.1340457585
H	2.5240878199	0.8973153384	-1.960324313
H	3.0049330013	2.5060292681	-1.3927438117
H	4.0333172202	1.1054983166	-1.0465645305
H	4.0333172202	1.1054983166	-1.0465645305

TS 6-31++G(d,p) 0003

E(UwB97XD) = -1036.74673942 A.U.

First frequency = -1530.5050 cm⁻¹

S	0.5262316606	-1.1466547778	1.1776526282
O	-0.5416937298	-2.1516353982	1.1469398074
O	1.2366164605	-0.9532850984	2.4507782987
N	-0.1332804176	0.2897555249	0.6174055718
C	0.8199684597	1.4153254706	0.6692873759
H	0.2599313942	2.313317101	0.3887026737
H	1.1845453851	1.5603099233	1.6949909103
C	1.9812180227	1.2141664538	-0.2993426028
H	2.1003791417	-0.0765122145	-0.2509280638
C	-1.5012943095	0.6019034889	1.0634493576
H	-1.46920808	1.2245716008	1.9675690639
H	-1.9890091696	-0.3368931606	1.3293296538
C	-2.2970746996	1.3078921225	-0.0341339363
H	-1.8679514395	2.2997557257	-0.2259546054
H	-3.3063619809	1.4856371146	0.3615374323
C	-2.3980863735	0.5444415411	-1.3611236372
H	-1.3782918998	0.4093308743	-1.7426842048
C	-3.0194069325	-0.8439426707	-1.1898517761
H	-4.0148112246	-0.7690536922	-0.7337977252
H	-2.4019960153	-1.4901172575	-0.5589065236
H	-3.132840818	-1.3366112208	-2.1613221758
C	-3.1796136194	1.3735520959	-2.3829315517
H	-2.7235878993	2.3588942866	-2.528988966
H	-4.2129747318	1.5275348353	-2.0483475418
H	-3.2140860485	0.8696126677	-3.3543667493
C	1.7385310656	-1.4175142666	-0.0741920519
H	2.6061434181	-1.9131041321	0.3596030007
C	1.2228778646	-1.93429163	-1.3902748504
H	0.9346388524	-2.9882771764	-1.3189234874
H	2.0054387544	-1.8447868548	-2.1483700233
H	0.351717596	-1.3634263929	-1.7229162433
C	3.2953431731	1.7913127316	0.1761145842
H	3.2296594656	2.8860779353	0.2441841153
H	3.5630214934	1.4105628235	1.1665082628
H	4.103987387	1.5512028125	-0.5202805697

C	1.6349218305	1.5116893565	-1.7429429987
H	1.5293417589	2.595595204	-1.8871680064
H	2.4175507328	1.1580596237	-2.4207363438
H	0.6895082204	1.0428636661	-2.0292595125
H	0.6895082204	1.0428636661	-2.0292595125

TS 6-31++G(d,p) 0004

E(UwB97XD) = -1036.74442403 A.U.

First frequency = -1540.9074 cm⁻¹

S	0.5634743149	-1.1906216687	0.6945165131
O	-0.1641419151	-2.3482254248	0.1635681549
O	0.3356499385	-0.8318897463	2.1024668909
N	0.2346627277	0.0930714412	-0.3304957347
C	0.86408615	1.3564210316	0.0971707583
H	0.4634419147	2.1399346137	-0.5565933111
H	0.5864611788	1.6110475264	1.1276453575
C	2.3805783006	1.2818219592	-0.0481961522
H	2.5714640288	0.0422962375	0.2894923706
C	-1.1358771823	0.1795749379	-0.8561696619
H	-1.3943044563	-0.8083341327	-1.2404891045
H	-1.0806872041	0.8581123533	-1.7152263039
C	-2.1845883192	0.6745709364	0.1407700016
H	-1.8327876054	1.6079531414	0.5975312697
H	-2.2867830148	-0.055631135	0.9546318257
C	-3.560801317	0.9239074064	-0.491742369
H	-3.4286904857	1.6480137511	-1.3089580192
C	-4.1686492357	-0.3536520357	-1.0803952815
H	-5.1722859152	-0.1587968788	-1.4722368126
H	-4.252769007	-1.128865739	-0.3089653167
H	-3.5686953978	-0.7592763437	-1.9005874911
C	-4.5088450563	1.5432793371	0.5386135857
H	-4.6733355116	0.8520883395	1.3741400866
H	-5.4830875053	1.7675414603	0.092051318
H	-4.1003776817	2.4736415382	0.9471759932
C	2.3093031459	-1.3219773323	0.4638012994
H	2.7770988152	-1.6030397782	1.4064671866
C	2.7666795554	-2.0369104199	-0.7786547219

H	3.8402264815	-1.8794431902	-0.912013186
H	2.2503182028	-1.6608483612	-1.6655267949
H	2.5860601182	-3.1145901592	-0.7074931667
C	3.147040932	2.1295915364	0.9409136228
H	2.8579080464	1.9013562301	1.9714043285
H	4.2248342635	1.9733043049	0.8383894534
H	2.9481689395	3.1958843337	0.7650129521
C	2.8613566365	1.369896979	-1.4809723551
H	2.7737744953	2.4039629987	-1.8415510909
H	3.9110965928	1.0737775777	-1.5675623354
H	2.2632632271	0.7324438402	-2.1384994106
H	2.2632632271	0.7324438402	-2.1384994106

TS 6-31++G(d,p) 0007

E(UwB97XD) = -1036.74433443 A.U.

First frequency = -1540.8976 cm⁻¹

S	0.5993331734	-1.2712903471	0.6676295253
O	-0.0892701202	-2.4616149047	0.1572099268
O	0.3825287533	-0.9133768006	2.077539883
N	0.2000389757	-0.0092492193	-0.3601317322
C	0.7792282035	1.283459517	0.0518159529
H	0.3420283599	2.042764957	-0.6070959597
H	0.4954199877	1.5355934935	1.0812546719
C	2.2966028265	1.2732305427	-0.1031348057
H	2.5445222767	0.0434173629	0.231191511
C	-1.1828048999	0.0227731559	-0.8597193586
H	-1.4241826939	-0.9771058178	-1.2286857066
H	-1.1582446433	0.6904186667	-1.726164169
C	-2.230377987	0.480074584	0.1565858987
H	-1.997271607	1.4978511016	0.4989964374
H	-2.1718054088	-0.1699197926	1.0378010556
C	-3.6655033287	0.4536259633	-0.387957425
H	-3.8709053797	-0.5665435385	-0.7426437021
C	-4.657955822	0.77188858	0.7335816707
H	-4.5515441172	0.072222536	1.5690826318
H	-5.6902899045	0.716002227	0.3729888149
H	-4.4912644051	1.7852628599	1.1190524522

C	-3.8600443473	1.4163446807	-1.564208009
H	-3.2450693134	1.1473384094	-2.4283526807
H	-3.5997093901	2.4404739964	-1.2688220379
H	-4.9042943326	1.4179458391	-1.8931754818
C	2.344529219	-1.3310986637	0.4071592752
H	2.838819484	-1.5924099718	1.3419939776
C	2.8118192181	-2.0247228293	-0.8436087383
H	2.6813237597	-3.1094706329	-0.7700834747
H	3.8748047165	-1.81917737	-0.9953086027
H	2.2637489954	-1.6719418842	-1.7210059174
C	3.0333275129	2.1516719251	0.8818234347
H	2.761036185	1.9099941029	1.9138299234
H	4.1160151473	2.04097998	0.7718109991
H	2.7885619051	3.2088601497	0.7089964485
C	2.7631200911	1.3824978264	-1.5392259595
H	2.1909993276	0.7172102294	-2.1923582165
H	2.6249009592	2.410999633	-1.8998211411
H	3.8248797652	1.1354455955	-1.6329079276
H	3.8248797652	1.1354455955	-1.6329079276

TS 6-31++G(d,p) 0016

E(UwB97XD) = -1036.74329748 A.U.

First frequency = -1531.0036 cm⁻¹

S	0.6023965185	-1.333865271	0.3341430314
O	0.4393636892	-1.8721805372	-1.0247451374
O	-0.0967802043	-2.0334981762	1.4185253123
N	0.1488135227	0.27452256	0.4291887497
C	0.7493809235	1.1192778113	-0.6207959353
H	0.5366531363	0.7207829158	-1.6208455956
H	0.2629667105	2.0987542043	-0.5461051222
C	2.2518124601	1.2649558006	-0.404451608
H	2.5203156213	0.0791689091	0.0405133258
C	-1.2579193892	0.545193636	0.7634422975
H	-1.2761455204	1.585812169	1.1009697442
H	-1.5194836121	-0.0777088118	1.6223283773
C	-2.2510597083	0.3202780898	-0.3778280945
H	-2.1487455388	-0.7115203106	-0.7344672756

H	-1.998440532	0.9734350134	-1.2246570356
C	-3.7124353954	0.566772409	0.0228564683
H	-3.9385054023	-0.0807528094	0.8821094488
C	-3.9654408982	2.0194836651	0.4398913884
H	-3.6887746178	2.7050849384	-0.3708265593
H	-3.3960387125	2.3023751048	1.3304125954
H	-5.0251899901	2.1774439737	0.665000901
C	-4.6446079517	0.1699038881	-1.1250536608
H	-4.4971021595	-0.876009334	-1.4135481943
H	-4.4551990063	0.7931082093	-2.0076992305
H	-5.6943690145	0.2995323432	-0.8421695032
C	2.3338894325	-1.1675617521	0.6447332192
H	2.4882165594	-0.9556794476	1.7025213323
C	3.2355589484	-2.1877832924	0.005370014
H	3.0585482559	-2.248911173	-1.0706494574
H	3.0906162249	-3.1856038969	0.4355320388
H	4.27580943	-1.8982265196	0.1744979643
C	2.6170167154	2.1787681645	0.7457620581
H	3.6792392208	2.0965740025	0.994776004
H	2.4146980652	3.2242680505	0.4763734526
H	2.0304595115	1.9388051632	1.6378586179
C	3.0520733083	1.4627636528	-1.6710681654
H	2.7979874659	2.4237769041	-2.1396975406
H	4.1252034272	1.4724117026	-1.4591355067
H	2.8478700843	0.6721264004	-2.3998586408
H	2.8478700843	0.6721264004	-2.3998586408

TS 6-31++G(d,p) 0017

E(UwB97XD) = -1036.74327744 A.U.

First frequency = -1535.9902 cm⁻¹

S	0.2876093985	-1.010550938	0.6740800409
O	-0.0817343729	-1.7615430915	-0.5344255393
O	-0.3990984743	-1.3652098331	1.9219689689
N	0.1055604993	0.6310862955	0.467668498
C	0.7367728042	1.171549622	-0.7468654634
H	0.3522688153	0.6717574048	-1.6450689482
H	0.4456637049	2.2259474553	-0.8082469288

C	2.2574144842	1.0671678208	-0.671921128
H	2.3702826797	-0.0519725505	-0.0294724918
C	-1.0872495009	1.3148008504	0.9901642172
H	-0.7414987384	2.2891512087	1.3534311782
H	-1.4289668089	0.7536652155	1.8612856468
C	-2.224158627	1.5325439394	-0.0116450669
H	-1.8577803401	2.151358689	-0.8407323103
H	-2.9862969973	2.1367896932	0.5003186737
C	-2.8862903174	0.2729535778	-0.5837427693
H	-2.104228655	-0.3491258052	-1.0374526436
C	-3.5831719968	-0.5542774225	0.5003527175
H	-2.881502412	-0.9058970077	1.2620964865
H	-4.0638408569	-1.435695763	0.0632240321
H	-4.3601032441	0.0408007063	0.9971442446
C	-3.8763509596	0.6608135311	-1.6856027307
H	-3.3815292367	1.2196853515	-2.4873732924
H	-4.6790114022	1.290525658	-1.2817247986
H	-4.3385899675	-0.2274377756	-2.1285643453
C	2.0455239226	-1.100431526	0.8324282495
H	2.33350151	-0.7113961676	1.8090185613
C	2.7059451822	-2.3724445926	0.3759589498
H	2.425294357	-2.6151770402	-0.6511976866
H	2.4386397791	-3.2215902244	1.0157054196
H	3.7906830522	-2.2465917048	0.4231990224
C	2.8870964557	2.081204291	0.259276068
H	2.8386835137	3.0844498565	-0.1853005982
H	2.3614305103	2.1103539347	1.2189782858
H	3.9394957719	1.8477574374	0.446553272
C	2.9426871936	0.8962752401	-2.0076850101
H	2.5341647818	0.043655265	-2.5591575484
H	2.8049853387	1.7930349387	-2.6278718325
H	4.0186037165	0.745403383	-1.8799106653
H	4.0186037165	0.745403383	-1.8799106653

TS 6-31++G(d,p) 0018

E(UwB97XD) = -1036.74514642 A.U.

First frequency = -1538.7552 cm^{-1}

S	0.4490636624	-1.5048189039	-0.3002078457
O	1.2404461607	-2.0703158422	-1.4035978337
O	-0.6938890428	-2.2950714056	0.1725908773
N	-0.1270930518	0.0170839864	-0.6691484868
C	0.9106132773	0.9391312964	-1.1644846767
H	1.445016978	0.4984908421	-2.0165796133
H	0.3922245326	1.8323209159	-1.5290337148
C	1.8763963629	1.3200354448	-0.0494382208
H	1.9365673247	0.1831299132	0.5679481029
C	-1.444768429	0.1103891786	-1.3172404505
H	-1.9576707005	-0.8442223077	-1.1903159677
H	-1.3155323261	0.2730979501	-2.3946037138
C	-2.2656561942	1.2399413726	-0.6967501245
H	-3.1853860247	1.3566146745	-1.2855953982
H	-1.7132689635	2.1831212748	-0.801653618
C	-2.6251139058	1.0270944208	0.7798746935
H	-1.7001290371	0.7623110683	1.3094603916
C	-3.1667484609	2.3237963045	1.385973023
H	-3.41249554	2.1916031875	2.444794173
H	-4.0794481239	2.6428795718	0.8674894408
H	-2.4344989662	3.1349332743	1.3070989813
C	-3.6218170051	-0.1199390074	0.9686601707
H	-4.5562392737	0.0888156716	0.4328005901
H	-3.8649726146	-0.2501868941	2.0283633072
H	-3.2221983358	-1.0707088736	0.603881118
C	1.5568792396	-1.0866421111	1.0124748399
H	0.9753596288	-0.8661382365	1.9076288809
C	2.7711870605	-1.9590723536	1.1762604025
H	3.3269084183	-2.0390692555	0.2393911355
H	2.5045194027	-2.9699810108	1.5056988368
H	3.4239572063	-1.5209461524	1.9355666366
C	1.2833198767	2.2699101383	0.9691389855
H	0.2938742564	1.9312597968	1.2913375083
H	1.9256239533	2.3588946188	1.8503252098
H	1.1720858074	3.2711114055	0.5309372795
C	3.2740806009	1.6557289473	-0.5155972117
H	3.9385926905	1.8344161895	0.3347046543
H	3.6961300657	0.8498893538	-1.124257667

H	3.2657056568	2.5683145363	-1.1277597139
H	3.2657056568	2.5683145363	-1.1277597139

TS 6-31++G(d,p) 0019

E(UwB97XD) = -1036.74341315 A.U.

First frequency = -1534.3419 cm⁻¹

S	0.5432844683	-1.3197590454	0.0331101003
O	0.3626622163	-1.5976436091	-1.3997022761
O	-0.2104764897	-2.1541715602	0.9762776606
N	0.188096015	0.2720096603	0.4090021714
C	0.8564641609	1.2482987848	-0.4721550935
H	0.6422186706	1.0433267139	-1.5285698836
H	0.4271176676	2.227995572	-0.2324259717
C	2.3604213074	1.2613430728	-0.2205340989
H	2.5496252068	0.0005074576	0.0039808808
C	-1.2046266179	0.5611921443	0.783594063
H	-1.179325868	1.5352470803	1.2854526166
H	-1.4963722495	-0.179090536	1.5301383395
C	-2.1979569395	0.5923991893	-0.3788839123
H	-2.2730714615	-0.4098318133	-0.8213792279
H	-1.8114594598	1.2548636891	-1.1633935541
C	-3.5984001577	1.0730134582	0.0261757301
H	-3.4942192049	2.0713015271	0.4757828717
C	-4.4880741299	1.204208012	-1.2128902697
H	-4.6227739786	0.228171854	-1.694649016
H	-4.0476836256	1.8847878955	-1.949234944
H	-5.4789846513	1.5867457563	-0.9471742793
C	-4.25137131	0.1499837938	1.0605097985
H	-3.6957586429	0.123363254	2.0027503666
H	-4.3112907526	-0.8753529897	0.6754884611
H	-5.2689922699	0.4837349248	1.2881980838
C	2.2778877726	-1.3206400386	0.3709985253
H	2.4305003734	-1.3133688618	1.4500210736
C	3.1242554453	-2.2636894093	-0.4395766905
H	2.9612098523	-2.1176770019	-1.5095779215
H	2.9108529056	-3.3115103027	-0.198496221
H	4.177668576	-2.0768245988	-0.2161278798

C	2.7571582208	1.9293314729	1.0785930025
H	3.8075623333	1.7376905947	1.3174176303
H	2.6232745845	3.0167796649	1.0004269413
H	2.1400374385	1.5703497633	1.9078639832
C	3.1943579431	1.6344869418	-1.4243386765
H	4.2620742317	1.5413579676	-1.2054978662
H	2.9585754827	1.0009589043	-2.2851607028
H	3.0048291325	2.6774168962	-1.7142955944
H	3.0048291325	2.6774168962	-1.7142955944

TS 6-31++G(d,p) 0029

E(UwB97XD) = -1036.74432661 A.U.

First frequency = -1532.2100 cm⁻¹

S	0.772412761	-1.4937291729	0.6337016976
O	-0.0816611007	-2.5366900159	0.0554269562
O	1.1070124298	-1.6080748064	2.0613941764
N	0.0434077617	-0.0226282574	0.289065404
C	0.7841345178	1.1289728678	0.8389593184
H	0.1508627585	2.0106204372	0.6928307022
H	0.936516978	1.0091588834	1.9199543295
C	2.1106742404	1.3232066256	0.1157040032
H	2.4397296716	0.0819687455	-0.065653443
C	-1.4188623817	0.0352486009	0.4451013579
H	-1.6745447137	0.4537050349	1.4290812074
H	-1.8020854573	-0.9854876934	0.4097388486
C	-2.0409563998	0.8653761413	-0.6750058243
H	-1.8723775383	0.3469833461	-1.6281650681
H	-1.520627673	1.8289635232	-0.7458770894
C	-3.5406609078	1.1307343457	-0.4878182927
H	-3.6718868794	1.6537908471	0.4704337321
C	-4.0544014523	2.048404629	-1.600386362
H	-5.1133437518	2.2862462582	-1.4563426904
H	-3.9491893865	1.5638471838	-2.5787375816
H	-3.4962974923	2.9903088908	-1.6294611584
C	-4.3564760512	-0.1651681809	-0.4384492934
H	-4.1972711099	-0.7541720919	-1.3501079238
H	-5.4264275453	0.0541500099	-0.3626219579

H	-4.0877024815	-0.7910819744	0.4179912233
C	2.2848906029	-1.2967440464	-0.2558543479
H	3.0924949383	-1.7732859508	0.2983553692
C	2.22027706	-1.542080469	-1.7391341812
H	2.0946357641	-2.6067447823	-1.9618088324
H	3.1512269091	-1.204066537	-2.2018948462
H	1.3902245238	-0.9962308994	-2.1949738108
C	3.1986886035	1.9479080935	0.95863076
H	2.9272528815	2.9770986834	1.2314731874
H	3.3579638221	1.3876092957	1.8850863241
H	4.1438938887	1.9898848	0.4097512377
C	1.9633872759	1.8964481165	-1.2777356313
H	1.1569464752	1.4002537358	-1.8254677831
H	1.7212288301	2.9663919573	-1.2171871432
H	2.8901296054	1.7954422311	-1.8504979196
H	2.8901296054	1.7954422311	-1.8504979196

TS 6-31++G(d,p) 0031

E(UwB97XD) = -1036.74406499 A.U.

First frequency = -1526.2020 cm^{-1}

S	0.7959959544	-1.4390704827	0.8566879003
O	-0.0016972682	-2.5899202214	0.4195372758
O	1.0853829849	-1.3245976457	2.2942694667
N	0.0290994597	-0.0666514091	0.2720008496
C	0.7139498799	1.1826497656	0.6566586153
H	0.053781002	2.0065266762	0.3654523623
H	0.8425078652	1.2331698488	1.7462197673
C	2.0512525899	1.3165045996	-0.0600343259
H	2.4310249476	0.0766888342	-0.0341990863
C	-1.4386769434	-0.0379559923	0.3886794396
H	-1.7222304221	0.5058802158	1.2983981764
H	-1.7968255011	-1.064749725	0.4906081096
C	-2.0580229183	0.5866762397	-0.8591877345
H	-1.7137911032	0.0091570356	-1.7252506301
H	-1.6845703949	1.6115351236	-0.9945924033
C	-3.592672863	0.619212336	-0.8432753871
H	-3.9497825521	-0.4064966624	-0.6732765655

C	-4.1453818097	1.5092968224	0.2750368879
H	-3.8751474574	1.1434271587	1.2700113466
H	-5.2382505084	1.5549537497	0.2274897569
H	-3.7621707101	2.5325230599	0.175169454
C	-4.1192880963	1.0827925878	-2.2042004028
H	-5.2139078205	1.0762603408	-2.2250836184
H	-3.7604921795	0.4357685651	-3.0114667386
H	-3.7858020483	2.105759694	-2.4180550424
C	2.3305437248	-1.3199205405	-0.0090808363
H	3.1350716739	-1.6708463184	0.6359543471
C	2.3271031825	-1.795077253	-1.4369000195
H	1.4936382525	-1.3626435434	-1.9964131926
H	2.249948618	-2.8857738904	-1.4939244135
H	3.2602606584	-1.4932626009	-1.9198389376
C	3.0904784001	2.1118941179	0.6962020824
H	2.772683019	3.159132456	0.7948984214
H	3.2439349987	1.7129265813	1.7036109546
H	4.0488644457	2.105602398	0.1689973443
C	1.9204829293	1.6560666424	-1.5296340563
H	1.6320154866	2.7099132793	-1.6447511824
H	2.8667511578	1.5088374962	-2.0587455338
H	1.1516418572	1.0433005649	-2.009217945
H	1.1516418572	1.0433005649	-2.009217945

TS 6-31++G(d,p) 0039

E(UwB97XD) = -1036.74323261 A.U.

First frequency = -1522.6565 cm⁻¹

S	0.6732064605	-1.5418055483	0.2196629523
O	1.0178375204	-2.2897801736	-0.9989560106
O	-0.2169715277	-2.2065402547	1.1789063171
N	-0.0194287675	-0.0578933362	-0.1390849069
C	0.7763197003	0.737175536	-1.0947998465
H	0.9857662452	0.1543218624	-2.0019528697
H	0.1554877493	1.5896226178	-1.3904250283
C	2.0642641844	1.2331370273	-0.4515156468
H	2.353680272	0.1918927358	0.2581571493
C	-1.4716312509	-0.0650570935	-0.3831564983

H	-1.8863641502	-0.9640982545	0.0750524928
H	-1.6695099793	-0.1196350861	-1.4632081918
C	-2.1192335746	1.1769684257	0.2243842181
H	-1.5689973535	2.0695327942	-0.0993504964
H	-2.0174362849	1.1251448782	1.3163561277
C	-3.5971051774	1.3497640258	-0.1502902267
H	-3.6613137368	1.4044334428	-1.2466220693
C	-4.455593588	0.1705922393	0.3186964298
H	-4.3639177253	0.0363179995	1.4035696573
H	-4.1668581114	-0.7688563731	-0.1625321681
H	-5.5117384909	0.3462609768	0.089933233
C	-4.13247224	2.6658549922	0.4199536667
H	-5.1737329702	2.8282731367	0.1232329604
H	-3.5431473515	3.5203820274	0.07071627
H	-4.0934952334	2.654878604	1.516022533
C	2.1729909057	-0.9935991674	0.9775306441
H	1.9511895645	-0.6376199351	1.9833566897
C	3.3753170593	-1.8821314785	0.8097823874
H	3.2553917277	-2.8340809023	1.3397958321
H	4.2505220918	-1.3759771857	1.2248481418
H	3.5620530618	-2.0977572607	-0.2444981452
C	1.8517869079	2.3342649843	0.5651914379
H	1.0443253745	2.077511945	1.2576117643
H	2.7620052947	2.5210337835	1.1427063718
H	1.5783989055	3.2688986318	0.0567742907
C	3.20490597	1.4513022153	-1.4185322212
H	4.1223430577	1.7210031291	-0.8873857528
H	3.3988993426	0.5551403941	-2.0162204408
H	2.9691797438	2.2712029827	-2.1112409834
H	2.9691797438	2.2712029827	-2.1112409834

TS 6-31++G(d,p) 0040

E(UwB97XD) = -1036.74373340 A.U.

First frequency = -1513.6381 cm⁻¹

S	0.4443140273	-1.1795278861	0.9548881365
O	-0.6132072696	-2.1397998178	0.6204362114
O	0.9364489774	-1.1741789728	2.3414235015

N	-0.115790143	0.3374530718	0.4952618111
C	0.8515027262	1.4136623452	0.791522368
H	0.3399219476	2.3594109298	0.5823738846
H	1.1134760493	1.411572796	1.8586255149
C	2.0961578461	1.3037159667	-0.0788365832
H	2.218895862	0.0159741621	-0.1251190978
C	-1.4985642909	0.6457613071	0.9140512934
H	-1.4713123693	1.1710545295	1.8776656179
H	-2.0240737228	-0.2970165486	1.0765821394
C	-2.2377101129	1.491224497	-0.1288600119
H	-1.5415622796	2.2223424803	-0.5586736788
H	-3.001870818	2.0732731509	0.4003878294
C	-2.9282343639	0.7224524831	-1.27026985
H	-3.362399624	1.4909765397	-1.9241749913
C	-1.958868743	-0.1094170074	-2.113839808
H	-2.4768975784	-0.5396212971	-2.977777869
H	-1.5373402393	-0.9322366665	-1.5282735366
H	-1.1295758022	0.5018292896	-2.4852388566
C	-4.0836489526	-0.1465946335	-0.762071873
H	-4.6340027242	-0.5833013429	-1.6018722503
H	-4.7896528396	0.4383187688	-0.1626325204
H	-3.7212526972	-0.9770340776	-0.1454975459
C	1.845451451	-1.332230724	-0.1080267233
H	2.6373573139	-1.858531441	0.4233576682
C	1.5699342227	-1.7430134806	-1.5287634214
H	1.2393029208	-2.7853928442	-1.5860220621
H	2.4861999523	-1.6422392992	-2.1163070105
H	0.7988264427	-1.1147529045	-1.9809066968
C	3.3554719183	1.8400906305	0.5628561546
H	4.2257463154	1.6655640183	-0.07641922
H	3.2716443763	2.9241878612	0.7210904292
H	3.5380206958	1.3734331963	1.5357339244
C	1.8736697303	1.7266342996	-1.5150936031
H	2.7057161427	1.4186272068	-2.1552475497
H	0.9493320379	1.2982962959	-1.9123511545
H	1.7906559685	2.8204789298	-1.57404901
H	1.7906559685	2.8204789298	-1.57404901

TS 6-31++G(d,p) 0041

E(UwB97XD) = -1036.74293750 A.U.

First frequency = -1519.0060 cm⁻¹

S	0.7184805862	-1.5827191753	0.2067150022
O	1.0283877706	-2.2823749527	-1.0494874005
O	-0.1048375903	-2.304553581	1.1843746077
N	-0.03553313	-0.1112931494	-0.0730478511
C	0.6921235443	0.7380655371	-1.0369737979
H	0.8775576177	0.1910897327	-1.9714035134
H	0.0330029009	1.5793784753	-1.2755541898
C	1.9924963534	1.254327115	-0.4363041523
H	2.3451645752	0.202265855	0.2264323138
C	-1.4952657467	-0.1648120009	-0.2690685969
H	-1.8710514771	-1.0838923602	0.1862375276
H	-1.718157392	-0.209362308	-1.3424949511
C	-2.1654637174	1.0337834294	0.3980774726
H	-1.7779999769	1.970107246	-0.0275167312
H	-1.8802674409	1.0272487089	1.456535825
C	-3.6960962642	1.0357027007	0.2808486827
H	-4.0657773971	0.0790361812	0.6765755318
C	-4.283686966	2.1597872725	1.1384880337
H	-3.9390104	3.1377084089	0.7803342014
H	-3.9829121215	2.0597191547	2.1866098079
H	-5.3777423582	2.1547255006	1.0973137233
C	-4.1694072555	1.1676355921	-1.1706280433
H	-5.2621092524	1.2173618591	-1.2174631595
H	-3.8522334056	0.3232831583	-1.7897574504
H	-3.7720624553	2.0857122396	-1.6212323762
C	2.2345047665	-1.0107274608	0.9128839136
H	2.0497657039	-0.6949689075	1.9393858247
C	3.4543410222	-1.8537013112	0.6588311377
H	4.3318973574	-1.3346340999	1.0523779946
H	3.5987307109	-2.0258887487	-0.4100284693
H	3.388068452	-2.8271966473	1.1582558508
C	1.794135302	2.31725592	0.6230741106
H	2.7235637691	2.5139030234	1.1657152816
H	1.4712003332	3.2581571721	0.1570520398

H	1.0262688896	2.0150203605	1.3416725409
C	3.0805515795	1.5364323965	-1.4465228115
H	3.2747686289	0.6640501531	-2.0783911535
H	2.7879749911	2.3671468538	-2.1037313702
H	4.0124328363	1.8208669072	-0.9493785723
H	4.0124328363	1.8208669072	-0.9493785723

TS 6-31++G(d,p) 0044

E(UwB97XD) = -1036.74327743 A.U.

First frequency = -1535.5923 cm^{-1}

S	0.258591358	-0.9218688351	0.7306299567
O	-0.1227949201	-1.601886873	-0.5155611993
O	-0.4177169059	-1.3465341733	1.9622311741
N	0.077745194	0.7291435488	0.6202670289
C	0.6994538994	1.3374988261	-0.5667482108
H	0.3064375785	0.8904282078	-1.4887391858
H	0.4096282297	2.3940334743	-0.5651732112
C	2.2204971734	1.2271210222	-0.5110463594
H	2.3367857062	0.0728217789	0.0651277802
C	-1.1091847999	1.3834030094	1.1915782684
H	-0.7584732217	2.3347991994	1.607164219
H	-1.4444397761	0.7736229051	2.0319794492
C	-2.2542916583	1.6598484402	0.2138876438
H	-1.8939628299	2.3248999612	-0.5813604618
H	-3.010981792	2.234550172	0.7663452786
C	-2.9234035324	0.4360718045	-0.4240313754
H	-2.1463224496	-0.1596443873	-0.9197392216
C	-3.6120793004	-0.4515962745	0.6166328474
H	-2.9043129171	-0.8475181955	1.3504859195
H	-4.0981216988	-1.3056872522	0.1336070653
H	-4.3835523561	0.1147033944	1.1539184811
C	-3.9224485282	0.8879142349	-1.492908855
H	-4.7206893804	1.49392525	-1.0462760118
H	-4.3897611699	0.0271915493	-1.9824447244
H	-3.4338290494	1.4917936764	-2.265310892
C	2.0176734342	-1.0229923715	0.8679422336
H	2.3149114843	-0.6912658465	1.8627365972

C	2.6717818961	-2.2674076819	0.333045123
H	3.7571172636	-2.1461503525	0.3785167158
H	2.3822543103	-2.4497450147	-0.7040987408
H	2.4080266402	-3.1518270518	0.9246626045
C	2.85988035	2.1852092341	0.4713704311
H	2.3424626143	2.1598704177	1.4356528381
H	3.9134217603	1.9400463947	0.6358737662
H	2.8094659505	3.2123903475	0.085557657
C	2.8940598894	1.1322724949	-1.8602599199
H	3.9707710513	0.9730413083	-1.7506055984
H	2.4794199833	0.3131513282	-2.4561521228
H	2.7525877332	2.0632722007	-2.426826176
H	2.7525877332	2.0632722007	-2.426826176

TS 6-31++G(d,p) 0045

E(UwB97XD) = -1036.74226919 A.U.

First frequency = -1494.6082 cm⁻¹

S	0.2235629944	-1.3855714007	-0.3764632467
O	0.8624358198	-1.9237410994	-1.5875329181
O	-0.9730321204	-2.0835573747	0.1091579717
N	-0.1966409926	0.2295407445	-0.5605836304
C	0.9175568371	1.0668247632	-1.0516066847
H	1.290374225	0.6806131892	-2.0106258463
H	0.4961007912	2.0602647462	-1.2396185061
C	2.044177443	1.17385746	-0.0317467965
H	1.9855082226	-0.0038710114	0.488708955
C	-1.4679776117	0.454542534	-1.2796591872
H	-2.0600221154	-0.4608368811	-1.2302455049
H	-1.2489152376	0.6394077757	-2.3397573993
C	-2.273814833	1.6226659394	-0.7098333806
H	-3.0269357963	1.8709862843	-1.4684107094
H	-1.6300807047	2.5073179131	-0.6205010509
C	-3.0041239489	1.3894725907	0.627212391
H	-3.6566073093	2.2638957458	0.7569130821
C	-3.9030371553	0.1493712836	0.5909719871
H	-4.5503989405	0.1495943436	-0.2933782072
H	-4.5445786704	0.1159884873	1.4776152768

H	-3.3080737637	-0.7702798371	0.5790113839
C	-2.06699303	1.3463560963	1.8376054668
H	-1.4573956724	2.2546300674	1.8941347621
H	-1.39132862	0.488079474	1.7832182411
H	-2.6445057772	1.2702543338	2.7654186444
C	1.4546014244	-1.2361848365	0.8795528327
H	0.9705417074	-1.0092926521	1.8293083601
C	2.5357469755	-2.2820601597	0.8870548668
H	3.0171718795	-2.3568685677	-0.0904690829
H	2.1438617002	-3.2700979535	1.1549799534
H	3.2892579173	-2.0081596957	1.6297092873
C	1.7397769127	2.0991686755	1.1266393925
H	0.7634963527	1.8705450735	1.5622172952
H	2.4997975143	2.0152591887	1.9091610624
H	1.7226370257	3.1425345003	0.7835185204
C	3.4199802853	1.3265895241	-0.639535726
H	4.1930771831	1.3151938565	0.1342108435
H	3.6313259711	0.5261446529	-1.3554037353
H	3.4993362249	2.2833993071	-1.1741370796
H	3.4993362249	2.2833993071	-1.1741370796

TS 6-31++G(d,p) 0046

E(UwB97XD) = -1036.74368063 A.U.

First frequency = -1543.9142 cm⁻¹

S	0.4296549302	-1.3493523727	0.3561681373
O	-0.0178681718	-2.5026473927	-0.4317759589
O	-0.0489186706	-1.243363297	1.7425195592
N	0.0376314742	0.0108452044	-0.5237849812
C	0.431772255	1.2747884339	0.121209403
H	-0.0149881979	2.0840533975	-0.4654074153
H	0.0312380573	1.3456101064	1.139617974
C	1.949845845	1.4233101486	0.1413846929
H	2.274305371	0.1888826979	0.3885272384
C	-1.1700630917	-0.043782867	-1.3632568068
H	-1.0411859474	-0.8750413468	-2.0601334895
H	-1.1503851882	0.8731799133	-1.9593453673
C	-2.5092142337	-0.2089059489	-0.640039628

H	-2.4959130084	-1.1664955599	-0.1060326333
H	-3.2830804267	-0.3017842447	-1.4155015681
C	-2.9199837236	0.9030057103	0.3347941351
H	-2.1267330456	1.014659668	1.0843302842
C	-3.1215332532	2.2484388535	-0.3680574797
H	-3.41659358	3.0211120454	0.3491605259
H	-3.9135515503	2.1702498277	-1.1230720121
H	-2.2160063013	2.5987119977	-0.87296394
C	-4.1953902919	0.4947021679	1.0777678694
H	-5.0244107879	0.3529968393	0.3733700685
H	-4.4946966675	1.2631085541	1.7980775357
H	-4.0518672272	-0.4438350066	1.6231316545
C	2.1911253878	-1.2069297808	0.3969198222
H	2.5588126136	-1.5283926123	1.3705269499
C	2.9251608811	-1.7032218828	-0.819694711
H	2.4845027949	-1.3077469583	-1.7385358898
H	2.9112083028	-2.796599433	-0.8758156732
H	3.9676665757	-1.3776175195	-0.7704114771
C	2.480609113	2.2579658384	1.284071395
H	2.1491133028	3.3007145957	1.1822425612
H	2.1239922777	1.8869600514	2.2499396595
H	3.5744349173	2.2588598827	1.2935489801
C	2.5529239933	1.7263450153	-1.2130506852
H	2.1211098769	1.0888316174	-1.9900086113
H	2.3534089027	2.7720536054	-1.4849366787
H	3.6377696178	1.5840861428	-1.2074284282
H	3.6377696178	1.5840861428	-1.2074284282

TS 6-31++G(d,p) 0057

E(UwB97XD) = -1036.74100275 A.U.

First frequency = -1605.7708 cm⁻¹

S	0.3877489784	-1.2902013523	0.5869464483
O	-0.3369691817	-2.3910861294	-0.0528680058
O	0.2321868286	-1.0901771204	2.0314126677
N	-0.0586366628	0.1075013223	-0.170101358
C	0.6165282941	1.3167696484	0.3140767176
H	0.1782959018	2.1646151684	-0.2237054543

H	0.3804726939	1.4521770584	1.3741872493
C	2.1353943272	1.2866220242	0.1144332524
H	2.3570869729	0.0073146574	0.2856111189
C	-0.7941463235	0.1222850295	-1.4362009619
H	-0.9879114303	-0.9155909174	-1.7129126346
H	-0.1584531563	0.5592197415	-2.2164943684
C	-2.1185280915	0.8851597147	-1.3770679396
H	-2.5226874018	0.8531808697	-2.3970061997
H	-1.9376852322	1.9469822305	-1.1592533484
C	-3.1671456354	0.3324544166	-0.3956890911
H	-3.0760314137	-0.7628202915	-0.3857540083
C	-2.9578443761	0.8429395968	1.0346001787
H	-1.9781174977	0.5645504914	1.4280916513
H	-3.7206977758	0.4341301115	1.7059459374
H	-3.0398485426	1.9370762212	1.06207818
C	-4.5781596309	0.6868346431	-0.876278633
H	-4.6997228766	1.775320057	-0.9427834877
H	-5.3369125056	0.3080774919	-0.183397602
H	-4.7813521721	0.2647611404	-1.8662109583
C	2.1282051413	-1.371204783	0.2746907707
H	2.6511739135	-1.779659405	1.138417349
C	2.5273369906	-1.8871304591	-1.0822150639
H	3.5843716734	-1.670892675	-1.2583582497
H	1.9471902188	-1.4146650325	-1.8801826465
H	2.3820194576	-2.9699113501	-1.1548746111
C	2.9121758031	2.018859005	1.1850159899
H	3.9898099628	1.8951453044	1.0431354047
H	2.6944339238	3.0954725244	1.1474649974
H	2.6489110671	1.6600662448	2.1848007976
C	2.5913103124	1.5679962627	-1.3021462394
H	2.4149240785	2.6234592715	-1.5508762342
H	3.6611037737	1.370237342	-1.4191247026
H	2.0523491168	0.9606412948	-2.0344568575
H	2.0523491168	0.9606412948	-2.0344568575

TS 6-31++G(d,p) 0058

E(UwB97XD) = -1036.74419712 A.U.

First frequency = -1524.8328 cm⁻¹

S	0.6203386734	-1.347276354	0.8971305902
O	-0.3670147573	-2.392415197	0.6120480353
O	1.2953113356	-1.3970287517	2.2030473462
N	-0.1478345593	0.125548969	0.6704404461
C	0.7289660129	1.2728375278	0.9830901487
H	0.1037559608	2.1703780817	0.9353398947
H	1.1243410845	1.1984727051	2.004581368
C	1.8620126115	1.3904109593	-0.0304548332
H	2.103977503	0.1349142743	-0.2431983274
C	-1.5438463406	0.1945363864	1.1560667644
H	-1.7044745976	1.2287654195	1.4692527676
H	-1.6824278687	-0.4202966689	2.0529636846
C	-2.5686627166	-0.1991560772	0.0927252914
H	-3.5644245751	0.0061055194	0.5106650944
H	-2.5092253426	-1.2790180943	-0.0728820237
C	-2.4275804405	0.5202123567	-1.2543111554
H	-1.444311285	0.2574971459	-1.6648247177
C	-3.4943182665	0.0170678046	-2.2300120213
H	-4.4995553671	0.2665723338	-1.8684137453
H	-3.4407264656	-1.0702789144	-2.3491744269
H	-3.3710707211	0.472816727	-3.2180533043
C	-2.4928788975	2.0434795274	-1.1205987766
H	-1.6646337867	2.4415240273	-0.5260358264
H	-3.4303124262	2.3516396642	-0.6410835864
H	-2.4450329203	2.5216457182	-2.1045276791
C	1.8712959462	-1.2419240579	-0.3429329746
H	2.7768408875	-1.7298738042	0.015292596
C	1.4360076554	-1.5322257014	-1.7536195412
H	1.2286115636	-2.5979987802	-1.8953744487
H	2.2321658601	-1.2439980974	-2.4450234605
H	0.5343416153	-0.9713932551	-2.0131692533
C	3.1330767371	1.9938910384	0.5220739859
H	3.4790743994	1.4536480947	1.4086254924
H	3.9303182146	1.9822454548	-0.2267889308
H	2.9646553683	3.0405005373	0.811446593
C	1.4230116902	1.9324188441	-1.3745400665
H	1.2209540014	3.0094694348	-1.2954143499
H	2.1986166497	1.7919140709	-2.1332658383

H 0.5059672678 1.4455587821 -1.7177487023
H 0.5059672678 1.4455587821 -1.7177487023

TS 6-31++G(d,p) 0060

E(UwB97XD) = -1036.74271188 A.U.

First frequency = -1542.0760 cm⁻¹

S 0.4168539937 -1.3306364458 0.2849757538
O -0.0126954322 -1.7014466291 -1.0714750317
O -0.0718029043 -2.1585075205 1.3941274673
N 0.0077824408 0.2419251428 0.6462233239
C 0.4632264239 1.2298527822 -0.3466192714
H 0.13304552 0.9619564081 -1.357762028
H -0.0106870529 2.1822822521 -0.0882261466
C 1.9809313185 1.3740690698 -0.3081054672
H 2.2960072407 0.13081423 -0.1220958427
C -1.2396185026 0.4670838784 1.3949693955
H -1.238371232 1.5318908967 1.6448226206
H -1.1548148551 -0.0778916992 2.3379731052
C -2.5427638079 0.0589512178 0.7030366113
H -3.3577833012 0.2434120401 1.4174713691
H -2.5197847447 -1.0249341566 0.5391823715
C -2.8773404254 0.7583580343 -0.6211601774
H -2.0375318351 0.60655432 -1.3106172514
C -4.1109101701 0.1076009259 -1.2536353397
H -4.9831373309 0.2130538447 -0.5966149595
H -3.9478641101 -0.9607916888 -1.4291148969
H -4.3549422007 0.5755783921 -2.2129800841
C -3.1011079987 2.2629193124 -0.4452907206
H -3.3369743553 2.7353942626 -1.4042923661
H -2.224122283 2.7733136683 -0.0355546049
H -3.9409317333 2.4472949922 0.2359745559
C 2.1811675211 -1.2013049032 0.2809498024
H 2.5336765248 -1.1718980764 1.3119395128
C 2.9254291174 -2.0921559034 -0.6758296736
H 3.9856731155 -1.8271496041 -0.6565302788
H 2.5522792992 -1.973022153 -1.6953403414
H 2.8384203651 -3.1493027653 -0.3993886019

C	2.4979713516	2.0799692241	0.9263644778
H	2.2588913714	3.151029417	0.8768343432
H	2.0389110354	1.6718230594	1.8320441862
H	3.5843606865	1.9830287479	1.0123727465
C	2.6010033532	1.8102349132	-1.6152099528
H	2.2874235397	2.8330671012	-1.8668946814
H	3.693027335	1.8061772947	-1.5516278382
H	2.2978490327	1.1563927105	-2.4390165758
H	2.2978490327	1.1563927105	-2.4390165758

TS 6-31++G(d,p) 0061

E(UwB97XD) = -1036.73995667 A.U.

First frequency = -1594.3294 cm⁻¹

S	0.3173823582	-1.2222308831	0.5236971877
O	0.1455814753	-1.9741669859	-0.7240665523
O	-0.4292792286	-1.6639898337	1.705786119
N	-0.0778977324	0.3540059448	0.2431611907
C	0.6499266827	0.9983422402	-0.8546199723
H	0.4675959419	0.4418521998	-1.7798473262
H	0.2128919603	1.994164044	-0.9880866786
C	2.1537565048	1.1028595392	-0.5920196987
H	2.3376140063	-0.0302792026	0.0288146907
C	-0.8825462364	1.1494387717	1.172086671
H	-0.2788487494	1.9913368446	1.532436979
H	-1.1092103336	0.5161086236	2.0315265749
C	-2.1864091363	1.6803194665	0.5738495576
H	-1.9722043573	2.3788624704	-0.2469745301
H	-2.650481693	2.2819481606	1.3659018787
C	-3.1843399833	0.6128676006	0.0905409489
H	-3.0968179905	-0.2578621649	0.7556453318
C	-4.6179096432	1.1441157398	0.1900887058
H	-5.339524289	0.3989302092	-0.1610054157
H	-4.7384161615	2.0431611462	-0.4273280715
H	-4.8760963846	1.4074039762	1.2213144127
C	-2.895283122	0.150531314	-1.3421194961
H	-2.97595203	0.996427879	-2.0367371726
H	-3.6183642696	-0.6099057213	-1.6562614021

H	-1.8950730291	-0.2768913321	-1.43833086
C	2.0578178177	-1.1313776063	0.8402718339
H	2.2115240959	-0.735794168	1.8451353656
C	2.9006477404	-2.3093780643	0.4338664856
H	3.9555046162	-2.0628656934	0.5806239285
H	2.7419480111	-2.5607099223	-0.6170483331
H	2.67554066	-3.1964029857	1.037407324
C	2.5405677649	2.1407034449	0.4407003849
H	1.9913102453	2.0015950217	1.3770270162
H	3.6100305936	2.0904581771	0.6658383353
H	2.3206576792	3.1503022277	0.0681656691
C	3.0031696483	1.0927623741	-1.8418685977
H	2.8251883454	2.0004020563	-2.4358393618
H	4.0680010591	1.0656827157	-1.5926010075
H	2.7720568132	0.2302503462	-2.4747299262
H	2.7720568132	0.2302503462	-2.4747299262

TS 6-31++G(d,p) 0062

E(UwB97XD) = -1036.74432659 A.U.

First frequency = -1532.2692 cm^{-1}

S	0.8311279351	-1.3155935055	1.1191227327
O	-0.0697020458	-2.4458861327	0.8690050962
O	1.2180733879	-1.0549046498	2.5139845211
N	0.1249657476	0.0332874855	0.4146824868
C	0.913994826	1.2645079017	0.6115820914
H	0.2969780015	2.0955693074	0.2533709627
H	1.1051888152	1.4335818191	1.6797496958
C	2.215832763	1.213249236	-0.177809537
H	2.5075616322	-0.0415803534	-0.0290475963
C	-1.3283308124	0.1798730286	0.5945914314
H	-1.5355210481	0.8547565415	1.4373793299
H	-1.737057597	-0.7996324264	0.8466179213
C	-1.9732702155	0.7002259275	-0.6876059135
H	-1.8540413471	-0.0596893055	-1.4711827249
H	-1.4332541508	1.5917979879	-1.0307440686
C	-3.4578716833	1.0558396098	-0.5324682123
H	-3.5394748892	1.8203251802	0.253635316

C	-3.9921488271	1.6589198508	-1.8342748743
H	-5.0387918791	1.9617148868	-1.7269004935
H	-3.9362921468	0.9270297909	-2.6492921125
H	-3.4133302585	2.5395974364	-2.1324099819
C	-4.3018669243	-0.1516320048	-0.1117152116
H	-5.3625471856	0.1155512776	-0.0646386471
H	-4.0152204752	-0.534156892	0.8726653367
H	-4.1921170792	-0.9680733486	-0.8361265515
C	2.3122093693	-1.4149076263	0.162976899
H	3.1289992621	-1.7526887782	0.7995478361
C	2.1840778977	-2.045911009	-1.1971339221
H	1.3501282249	-1.6145618979	-1.7567723117
H	2.0245622861	-3.1265260996	-1.1216127043
H	3.104079922	-1.8753168707	-1.7624339694
C	3.3504568829	2.003774835	0.4323181264
H	4.2743997844	1.8655725665	-0.1366035172
H	3.1146759138	3.0769626352	0.4269696208
H	3.5319985253	1.7067579959	1.4698378712
C	2.0285798398	1.3972268423	-1.6688026286
H	1.1897813096	0.7999680408	-2.0379425166
H	1.8148617783	2.4518596881	-1.8905218073
H	2.9297327013	1.1154655888	-2.2216539658
H	2.9297327013	1.1154655888	-2.2216539658

TS 6-31++G(d,p) 0064

E(UwB97XD) = -1036.74406504 A.U.

First frequency = -1526.1515 cm^{-1}

S	0.8406582674	-1.2340294385	1.2358834832
O	0.0050941956	-2.4305638816	1.0875206964
O	1.173471719	-0.8078091282	2.6037509595
N	0.0884670136	-0.0068552802	0.3746085383
C	0.8119854581	1.2769877443	0.4521489788
H	0.1624835652	2.0327597271	-0.0021117723
H	0.9727280012	1.5673554586	1.499082249
C	2.1309359753	1.2083912434	-0.3065371294
H	2.4832758188	-0.0041831683	-0.0106260532
C	-1.3743402182	0.0889622192	0.5153944456

H	-1.619376458	0.8311171339	1.2853999472
H	-1.7524424913	-0.8780895657	0.8542360453
C	-2.0149904898	0.4345247433	-0.8266483233
H	-1.7083897766	-0.3321064231	-1.5480156202
H	-1.6229840565	1.3919676916	-1.1978240521
C	-3.5474704652	0.512660928	-0.7835596202
H	-3.9221822146	-0.4383601162	-0.3790160853
C	-4.048335134	1.646062468	0.1180447131
H	-5.1408470361	1.7102951558	0.0864292695
H	-3.6457168844	2.6096946101	-0.2183010523
H	-3.7579405024	1.5054503301	1.163396581
C	-4.102215002	0.6735596879	-2.2015562814
H	-3.7809699876	-0.1479064772	-2.8504390676
H	-3.7523757811	1.6126979309	-2.6476942261
H	-5.1968616277	0.6931436383	-2.1955130506
C	2.3521441834	-1.3559825157	0.3308276988
H	3.1666670275	-1.5757031507	1.0198553668
C	2.297221391	-2.1394974939	-0.9527395986
H	1.4580017272	-1.8204446168	-1.5761415631
H	2.1940372119	-3.2124900316	-0.7607406766
H	3.2227181419	-1.9804200666	-1.5124320677
C	3.2089985453	2.1235463424	0.227131534
H	2.9178815239	3.1747686922	0.0943703238
H	3.3820652852	1.9570455389	1.2948026239
H	4.1515776088	1.9716651018	-0.3066898967
C	1.9658960754	1.2126538185	-1.8114857164
H	1.1701668376	0.5297508312	-2.1230255449
H	1.6978908665	2.2214049437	-2.1544905176
H	2.8931466622	0.9236852614	-2.3152329903
H	2.8931466622	0.9236852614	-2.3152329903

TS 6-31++G(d,p) 0069

E(UwB97XD) = -1036.73986289 A.U.

First frequency = -1583.8080 cm^{-1}

S	0.2835377446	-1.3207156292	0.3498292667
O	0.2615824192	-1.9205518104	-0.9877365607
O	-0.5223262185	-1.9437758993	1.4040892747

N	-0.2076062915	0.2509306622	0.2008788738
C	0.566453377	1.0387814482	-0.7681326383
H	0.4505835915	0.5773477196	-1.7532366167
H	0.1006433072	2.0279228379	-0.8233036716
C	2.0540589912	1.1681633835	-0.4240850234
H	2.2536087564	0.0075310299	0.1352820789
C	-0.9687234002	0.9210719753	1.2618342354
H	-0.3094066256	1.5735175898	1.8480703756
H	-1.3350218102	0.1440918873	1.9333729236
C	-2.1437221221	1.7521563404	0.7407436089
H	-1.7723598182	2.5959831827	0.1454281553
H	-2.6013106314	2.1984172392	1.6331391421
C	-3.2384576191	1.0179988717	-0.0567367136
H	-4.077404382	1.7250029578	-0.1140613061
C	-2.8326367625	0.6955010206	-1.5002758985
H	-2.445445569	1.5850598249	-2.0101360769
H	-3.6985649573	0.3355750819	-2.0664989706
H	-2.0606573269	-0.0778182243	-1.5354604801
C	-3.7424990652	-0.2343799296	0.6659071629
H	-4.6142653556	-0.6506527219	0.1505407056
H	-4.0364205967	-0.0084642964	1.6973464154
H	-2.9720603593	-1.0122734329	0.697618827
C	1.9828654615	-1.1732417913	0.8279087158
H	2.0307468478	-0.8654931016	1.8734411289
C	2.9252567919	-2.2626134822	0.3931938886
H	2.8693381961	-2.4214272622	-0.6859101683
H	2.7039801709	-3.2129138277	0.8929179825
H	3.9478524581	-1.9771088513	0.6533963995
C	2.3739557673	2.1618247559	0.6738235261
H	3.4402449497	2.1445323236	0.9182119958
H	2.1176526555	3.180355261	0.3523700417
H	1.8157389864	1.9507223349	1.590473475
C	2.9556477683	1.2489839781	-1.6354041827
H	4.0095025681	1.2425856054	-1.341915273
H	2.7800266519	0.4132354391	-2.3199065455
H	2.7721226617	2.179787394	-2.1905646557
H	2.7721226617	2.179787394	-2.1905646557

TS 6-31++G(d,p) 0074

E(UwB97XD) = -1036.74402483 A.U.

First frequency = -1523.1104 cm⁻¹

S	0.7670119547	-1.635921636	0.5170022152
O	0.0465241268	-2.7363751861	-0.1320546952
O	1.2217705448	-1.8497195162	1.8995381485
N	-0.2166755647	-0.2802783357	0.3992571453
C	0.3681917428	0.9154885459	1.0403119567
H	-0.3942844751	1.6992072525	0.9934873918
H	0.5759898567	0.7203720482	2.1011693928
C	1.626940607	1.3864023845	0.3197539584
H	2.1235557288	0.2469974433	-0.0420528279
C	-1.6492658032	-0.5245197041	0.6764648882
H	-1.9313702796	0.0351607712	1.5749141928
H	-1.7964540705	-1.5813543478	0.9087058861
C	-2.5283575265	-0.1629663381	-0.5184291753
H	-3.5544757464	-0.4852937154	-0.2917991366
H	-2.1891356454	-0.7629778364	-1.3713622255
C	-2.5529800425	1.318719165	-0.9173039289
H	-1.5170938959	1.6502770677	-1.0633611255
C	-3.2830666359	1.4906832809	-2.2519098445
H	-3.294607053	2.5404653766	-2.5630074399
H	-4.3237069685	1.1536535586	-2.1689732197
H	-2.8028335539	0.9069001228	-3.0442140329
C	-3.1956453505	2.1977479309	0.1596766766
H	-2.6784142207	2.1280184833	1.1222158395
H	-4.239098274	1.9017790019	0.3229626332
H	-3.188156314	3.2500994209	-0.1421157025
C	2.1587244979	-1.0985324826	-0.4237725591
H	3.067738977	-1.5095600177	0.0134169956
C	2.0161121112	-1.1615692439	-1.9203270514
H	1.0681607977	-0.7265158135	-2.2472010524
H	2.0611075569	-2.1947614857	-2.2801832294
H	2.8318112639	-0.6022343906	-2.3860900085
C	2.6452725186	2.0458814394	1.2220203369
H	2.2424067251	2.9820060767	1.6328830881
H	2.9111572988	1.3990382524	2.0636569404

H	3.5567266628	2.2923402982	0.6698589763
C	1.3612323959	2.1098597786	-0.9836591148
H	0.6727821155	1.5455309505	-1.6187666661
H	0.9084885154	3.090873643	-0.78436615
H	2.2887844422	2.2747142874	-1.5398226372
H	2.2887844422	2.2747142874	-1.5398226372

TS 6-31++G(d,p) 0077

E(UwB97XD) = -1036.74258464 A.U.

First frequency = -1517.2076 cm⁻¹

S	0.5137299688	-1.4501514381	-0.4451048146
O	1.3204481606	-1.8278090572	-1.6157810682
O	-0.5692629443	-2.3635412373	-0.0656866041
N	-0.1660415823	0.0678832824	-0.6385708862
C	0.821423367	1.0842179611	-1.0587671041
H	1.3439121333	0.7712469357	-1.9723578634
H	0.2576150961	1.9922258886	-1.296271357
C	1.8140396946	1.3795722807	0.0599030472
H	1.9347784534	0.1959763965	0.5637276076
C	-1.4826221613	0.0917094555	-1.3146746524
H	-1.5390620024	-0.669409047	-2.1019673706
H	-1.5396617419	1.0577964231	-1.8214032788
C	-2.660439133	-0.0640917516	-0.3519244775
H	-2.7121439732	-1.1040540133	-0.0171117267
H	-3.575684265	0.1330260329	-0.927938903
C	-2.6271290461	0.8535790382	0.8761433478
H	-1.7252339163	0.601516235	1.4489192308
C	-2.5532428928	2.3353343544	0.500060314
H	-1.6327486266	2.5776096748	-0.0400971544
H	-2.5796794434	2.9655104381	1.3952471428
H	-3.4016779291	2.6171593842	-0.1359984407
C	-3.8434142914	0.5821136395	1.7651190164
H	-4.7730004755	0.8290830486	1.2373933272
H	-3.8065576041	1.1851688998	2.6784743865
H	-3.8933151982	-0.4722373875	2.0571957023
C	1.6139728458	-1.1225409084	0.896546173
H	1.0345156855	-1.0129129015	1.8131142146

C	2.8641510939	-1.9562528382	0.9638726208
H	3.4126870862	-1.9189793541	0.0201374275
H	2.6416634277	-3.0050907996	1.1919895181
H	3.506580681	-1.5698769855	1.759155774
C	1.2335975441	2.2013215595	1.1912976516
H	1.0622382094	3.2343871929	0.8593546704
H	0.2749888763	1.7910177543	1.5222444171
H	1.9143876224	2.2322366511	2.0471936146
C	3.1832293262	1.8066252741	-0.4168396394
H	3.6063710409	1.0800396967	-1.1175332472
H	3.1252008378	2.774933505	-0.9331667476
H	3.8727720173	1.9217895157	0.4244609755
H	3.8727720173	1.9217895157	0.4244609755

TS 6-31++G(d,p) 0078

E(UwB97XD) = -1036.74323252 A.U.

First frequency = -1522.6617 cm⁻¹

S	0.7340681268	-1.6201724854	-0.4359398389
O	1.1599342045	-1.875725603	-1.820354465
O	-0.2095186453	-2.5754642239	0.156942227
N	0.0542154133	-0.096991466	-0.2678217923
C	0.9023901682	0.9798848917	-0.8152919435
H	1.1726243307	0.7663209956	-1.8583031601
H	0.2949794433	1.8912268808	-0.8153576062
C	2.1437379997	1.1851990779	0.0423100027
H	2.395912346	-0.0480453656	0.3373954194
C	-1.3796610307	0.0088470374	-0.5861988451
H	-1.8154982105	-0.9888068529	-0.5157269857
H	-1.5087148732	0.3567595299	-1.6210591994
C	-2.0737665254	0.9521928095	0.3932958126
H	-1.511593793	1.8927389348	0.453048967
H	-2.0397896019	0.5027759412	1.3944590506
C	-3.5267556558	1.2728607043	0.0186605079
H	-3.5229936318	1.7257041444	-0.9833231129
C	-4.4034526901	0.0172835739	-0.0296200624
H	-4.0779315252	-0.6854046919	-0.8027802315
H	-5.4446575058	0.2807681738	-0.2419934287

H	-4.3784446137	-0.5058886267	0.9342519565
C	-4.1069973824	2.2973003178	0.9973018712
H	-3.5037500326	3.2110737502	1.0217368271
H	-4.1364403137	1.885526702	2.0134625447
H	-5.1289459762	2.5731826262	0.7177382859
C	2.179277875	-1.411528043	0.5600830995
H	1.89223673	-1.4448474941	1.6108446973
C	3.396304391	-2.1962304064	0.1522815199
H	3.2501815782	-3.274107365	0.2876886305
H	4.2397971257	-1.8917945209	0.7770118468
H	3.6508107028	-2.0134349082	-0.8939912668
C	1.8597296264	1.8409058323	1.3767458603
H	1.6116797581	2.9010165718	1.2304382999
H	1.0124532804	1.3613996662	1.876301164
H	2.7305697345	1.788737042	2.0369123391
C	3.3410662313	1.7239828865	-0.7059557897
H	3.5787572611	1.1059780258	-1.5774731414
H	3.1431272658	2.7442866771	-1.0629552094
H	4.2214042369	1.7656378586	-0.0580242954
H	4.2214042369	1.7656378586	-0.0580242954

TS 6-31++G(d,p) 0079

E(UwB97XD) = -1036.74293743 A.U.

First frequency = -1519.0652 cm⁻¹

S	0.7521251725	-1.6847471193	-0.1628465288
O	1.134186089	-2.1014400804	-1.52077533
O	-0.1294202277	-2.5879530492	0.5866721669
N	0.0195696013	-0.1763272169	-0.1604308537
C	0.8051180362	0.8498884553	-0.8744654546
H	1.0441857781	0.5147124834	-1.892911223
H	0.1633617543	1.7327969397	-0.9627248047
C	2.0689353885	1.2044896402	-0.1029044239
H	2.3791680291	0.028940317	0.3356009348
C	-1.4260554675	-0.1642278793	-0.4470310679
H	-1.8303827319	-1.1540857249	-0.2235915101
H	-1.584861554	0.0271772014	-1.5157007023
C	-2.1319135925	0.8722391292	0.4238170895

H	-1.7173046467	1.8722761317	0.2341226403
H	-1.910547648	0.6329362757	1.4704536133
C	-3.6527900178	0.923053623	0.2214567485
H	-4.0479181091	-0.0906839617	0.378568481
C	-4.2877569086	1.8442704775	1.2667087434
H	-4.0504023172	1.515574503	2.2838909969
H	-5.3774059742	1.8650533562	1.1622532351
H	-3.919841175	2.8710443372	1.149319258
C	-4.038123862	1.3726869472	-1.1918954814
H	-3.6121276	2.3601344038	-1.4093043979
H	-5.1259363884	1.4483065497	-1.2899262934
H	-3.6867398961	0.6771548235	-1.9597601187
C	2.225038544	-1.3017553347	0.7360356681
H	1.9805854816	-1.212107885	1.7942154609
C	3.4556893974	-2.0885488737	0.3760146115
H	3.3575116278	-3.1457551579	0.6483828928
H	4.3096550695	-1.6800780961	0.9221915678
H	3.6627557702	-2.0281874094	-0.6947041463
C	1.810885159	2.0165563315	1.1482560353
H	1.5184685761	3.0406915425	0.8791876505
H	1.001074379	1.5780693325	1.7392578999
H	2.707056346	2.077216223	1.7728883502
C	3.2155552853	1.6814125645	-0.9641766305
H	3.44460415	0.9631792668	-1.7577166632
H	2.9644729515	2.6388054175	-1.4416367033
H	4.1171113711	1.837534402	-0.3647760075
H	4.1171113711	1.837534402	-0.3647760075

TS 6-31++G(d,p) 0083

E(UwB97XD) = -1036.74174708 A.U.

First frequency = -1595.4871 cm⁻¹

S	0.5347617842	-1.480426708	0.4275846944
O	0.512653835	-2.2150503774	-0.8409639277
O	-0.1422408016	-2.067231117	1.587832476
N	-0.1385403943	0.0071617249	0.1692548037
C	0.5123293594	0.7997289487	-0.8814282446
H	0.4895322288	0.2239126724	-1.8112486954

H	-0.1025255654	1.6916522484	-1.0426473232
C	1.9539880966	1.1862323162	-0.5444319292
H	2.3257601359	0.0779360987	0.038166418
C	-0.9562580821	0.6509572639	1.2083816484
H	-0.7338898441	1.721199336	1.1752888756
H	-0.6472589822	0.2938066822	2.1941725811
C	-2.4501767618	0.3966778203	1.0148366663
H	-2.9877703484	0.8670123142	1.8503863739
H	-2.620626677	-0.6831993547	1.0952432036
C	-3.0292063475	0.9062260327	-0.3115518192
H	-2.4094316184	0.5013219775	-1.1234700442
C	-4.453501053	0.3788123653	-0.5038629019
H	-5.1102490819	0.7376588397	0.2983514758
H	-4.4750539065	-0.7158613681	-0.4919352027
H	-4.874087221	0.7160908431	-1.4570022854
C	-3.0109805399	2.4353737726	-0.4022042061
H	-3.4143745327	2.7729369714	-1.3623605434
H	-2.0019465045	2.8500217542	-0.3070789179
H	-3.6253217889	2.874050918	0.3937431211
C	2.2289917477	-1.0979390265	0.7849701991
H	2.2986291413	-0.7374493476	1.8121442795
C	3.2736937899	-2.0840347646	0.3372565482
H	4.2657315973	-1.6618157659	0.5177763637
H	3.1742972834	-2.3037069528	-0.7279638849
H	3.2039724269	-3.0277294022	0.8906119052
C	2.0951276114	2.2316296541	0.5421374292
H	1.5745574555	1.9375027113	1.4588015725
H	3.14748395	2.3969026732	0.7911419487
H	1.672775798	3.189288659	0.2082668623
C	2.8336993054	1.3975544504	-1.7549832501
H	2.5053373527	2.2813782855	-2.320003428
H	3.8740943644	1.5631615274	-1.4602527825
H	2.7964900483	0.5376421775	-2.431055178
H	2.7964900483	0.5376421775	-2.431055178

TS 6-31++G(d,p) 0085

E(UwB97XD) = -1036.74071217 A.U.

First frequency = -1586.6414 cm^{-1}

S	0.8023300166	-1.7618219536	-0.0367457237
O	1.6419386798	-2.2349342276	-1.1389276913
O	-0.1001768545	-2.71216265	0.6174695442
N	-0.1359699453	-0.5127052446	-0.6390504097
C	0.6895505211	0.5307911711	-1.2841906139
H	1.2275315614	0.0419813552	-2.0987102032
H	0.0043466173	1.2483105714	-1.7438166251
C	1.6888805685	1.2442254566	-0.3622503582
H	1.9237093522	0.2823703015	0.4884268277
C	-1.2474828988	-0.0940872714	0.241508363
H	-0.873818702	0.3435067479	1.1767289181
H	-1.7962383985	-1.0006227379	0.5037576971
C	-2.1928870606	0.8765633994	-0.4584113059
H	-2.3993263242	0.4956951388	-1.4659120672
H	-1.7192299148	1.8603330892	-0.5747639242
C	-3.5188615581	1.0694156752	0.2921835945
H	-4.0023745034	0.0865379451	0.3801346881
C	-3.3086440163	1.627654865	1.7035952588
H	-4.270406523	1.8214145675	2.1892543327
H	-2.755594357	2.5745562506	1.6636125253
H	-2.7507753559	0.9370282793	2.3433037079
C	-4.4451451841	1.9826934566	-0.514681108
H	-4.0059275366	2.9822884648	-0.6199447379
H	-5.4149466651	2.0934018163	-0.019097157
H	-4.6209606089	1.5841041022	-1.5193014184
C	1.8520828503	-0.9504854664	1.1418621744
H	1.2822742152	-0.7390158767	2.0472615571
C	3.2377462751	-1.5077303839	1.3289098821
H	3.2157746712	-2.4962311801	1.8019662202
H	3.8084314021	-0.8378728378	1.9772523798
H	3.7578372767	-1.5970501475	0.3726627036
C	1.1354970926	2.4032091789	0.4427839432
H	0.2433220694	2.1328520282	1.0128452359
H	1.8839266011	2.7831207777	1.1445849066
H	0.8606682635	3.2272081454	-0.2300898979
C	3.0173723111	1.5359313726	-1.0274586216
H	2.8881741841	2.2658390485	-1.8387617534
H	3.7306769451	1.9582387534	-0.313413829

H	3.453633093	0.6307803613	-1.4613156661
H	3.453633093	0.6307803613	-1.4613156661

TS 6-31++G(d,p) 0086

E(UwB97XD) = -1036.74281446 A.U.

First frequency = -1506.2510 cm⁻¹

S	0.6535884631	-1.6606495527	-0.1563657248
O	1.1929916732	-2.057139063	-1.4662752087
O	-0.161538295	-2.653838242	0.5531985695
N	-0.2735240953	-0.2654679837	-0.2684125711
C	0.4259957614	0.844202505	-0.9494804254
H	0.7582631503	0.5343606382	-1.9498347393
H	-0.3098663474	1.6431567844	-1.0823151615
C	1.5984001256	1.359633097	-0.1243497475
H	2.0216180113	0.2469698514	0.3718672373
C	-1.6736882403	-0.494136111	-0.6916170724
H	-1.8426891399	-1.5666820172	-0.808133024
H	-1.8186810041	-0.0458572599	-1.6808334701
C	-2.6737504993	0.0433867383	0.3296654802
H	-2.4686444983	-0.4527219083	1.285715681
H	-3.6774329611	-0.2762494052	0.0155330724
C	-2.685228927	1.5639298548	0.5383838239
H	-1.663048496	1.8855430703	0.7751202625
C	-3.1542906815	2.3157628558	-0.7107781665
H	-2.5276561533	2.1104248243	-1.5848636061
H	-3.1393077148	3.3973498907	-0.5420196889
H	-4.1816994946	2.0291438458	-0.9663704155
C	-3.5674496663	1.9208522271	1.7377020628
H	-3.5759161588	3.0015975162	1.9133367571
H	-3.2121762371	1.4312379538	2.6504926808
H	-4.6023005708	1.6006677415	1.5646170409
C	1.9894709992	-1.0703511487	0.8360158232
H	1.6478066135	-0.9621234673	1.8650889176
C	3.3274795066	-1.7222257073	0.6171292316
H	3.6173562987	-1.6828436546	-0.435122657
H	3.3260634407	-2.7711842869	0.9352649593
H	4.0795321542	-1.1941132238	1.2085855307

C	1.1950056974	2.1644321082	1.0930520915
H	0.4548185071	1.6263178231	1.6928794791
H	2.0614620169	2.3812528625	1.7248004246
H	0.7527746124	3.1222233898	0.7868379802
C	2.7221484893	1.9481510502	-0.9463349536
H	2.3848141807	2.8585576232	-1.4611517017
H	3.5697246199	2.2222302291	-0.3116413936
H	3.0706050886	1.2440332108	-1.708305816
H	3.0706050886	1.2440332108	-1.708305816

TS 6-31++G(d,p) 0094

E(UwB97XD) = -1036.74341316 A.U.

First frequency = -1534.3644 cm⁻¹

S	0.443385018	-1.2014066253	0.3056710507
O	0.2613928752	-1.5213652102	-1.1181633142
O	-0.3361157616	-1.9842229669	1.2718716705
N	0.1289299932	0.4106693978	0.6274503704
C	0.826544584	1.3394833101	-0.2819173944
H	0.6113267037	1.1055415304	-1.3320979334
H	0.4222895111	2.3375010323	-0.0766087919
C	2.329266321	1.3212099294	-0.0233418624
H	2.4840833868	0.063912889	0.2433855128
C	-1.2572424721	0.7485335586	0.9852322054
H	-1.2083524552	1.7376469518	1.4548582588
H	-1.5715792811	0.0412448416	1.7542565489
C	-2.24449722	0.7673195952	-0.1826766604
H	-2.3444473271	-0.2467621298	-0.592024988
H	-1.8371942188	1.3927879841	-0.98678074
C	-3.6333117795	1.298104779	0.1991129695
H	-3.5044306983	2.3077230341	0.6158147269
C	-4.514021427	1.4114360495	-1.04809102
H	-4.052669639	2.0553094845	-1.8043435258
H	-5.4955363022	1.82859531	-0.8001968559
H	-4.672553884	0.4238149795	-1.4979296357
C	-4.3149091253	0.4277040483	1.2602580608
H	-3.7641772115	0.4179549588	2.2056859667
H	-4.4003771614	-0.6079939883	0.9092987916

H	-5.3242724716	0.7955947333	1.4715075303
C	2.1759402826	-1.2368698852	0.6520947475
H	2.3242244543	-1.1981653913	1.7310509091
C	3.0004116597	-2.2279750932	-0.1229417197
H	2.8457607941	-2.1129196542	-1.1979546964
H	2.758347725	-3.2613380515	0.1511977569
H	4.0574626001	-2.0616683499	0.0995739899
C	2.7381952338	2.0209585955	1.2551198818
H	2.6334942794	3.1083908306	1.1406283605
H	2.1083634196	1.7058783343	2.0926357644
H	3.7821589513	1.8096858483	1.505351629
C	3.1777585555	1.6323612908	-1.2345719432
H	4.2417243073	1.518492711	-1.0074305562
H	2.9288922293	0.9771571913	-2.0752504364
H	3.0170552985	2.669763704	-1.5596417644
H	3.0170552985	2.669763704	-1.5596417644

TS 6-31++G(d,p) 0095

E(UwB97XD) = -1036.74368071 A.U.

First frequency = -1544.0625 cm⁻¹

S	0.4245391635	-1.4183120729	0.0072420271
O	0.0059372487	-2.4665320741	-0.9293643781
O	-0.1094673829	-1.4738316931	1.376182319
N	0.0723977784	0.0395777844	-0.7198119816
C	0.4440188879	1.2150819474	0.0857685654
H	0.0238445791	2.0916462575	-0.4179295348
H	0.0028650891	1.1678863875	1.0886544131
C	1.9604684943	1.3483470001	0.1837528586
H	2.2709800165	0.0908030063	0.2954416875
C	-1.1008892893	0.0942080982	-1.6067590113
H	-0.9463339831	-0.6489777157	-2.3922763436
H	-1.0549745122	1.0755167023	-2.0878516815
C	-2.4683994148	-0.1460089238	-0.9618859293
H	-2.4793498351	-1.1607018419	-0.5464735949
H	-3.2108531936	-0.1393824977	-1.7727835357
C	-2.9145326551	0.8443379682	0.1223452001
H	-2.1514995864	0.8593425793	0.9104277443

C	-3.0839265164	2.2657401016	-0.4214658367
H	-3.8455738404	2.284626778	-1.2107632591
H	-2.158004797	2.6668563037	-0.8449929914
H	-3.4048831064	2.9493067195	0.3711323468
C	-4.2197623618	0.3598454828	0.7603251538
H	-5.0204336021	0.3099173072	0.0120167778
H	-4.5453025015	1.0387416867	1.5553109985
H	-4.1008812806	-0.6383286361	1.1943625884
C	2.1833347377	-1.2953729122	0.1347996313
H	2.5102929349	-1.7326970899	1.0772913075
C	2.9645807525	-1.649968526	-1.1018071608
H	2.9490731323	-2.7288127498	-1.288006345
H	4.0053459968	-1.3412055408	-0.9724458371
H	2.5631341229	-1.1446332838	-1.984034963
C	2.4471401999	2.0377332944	1.4375369895
H	2.1229787272	3.087691988	1.4470733802
H	2.0508513037	1.5576723189	2.3376590049
H	3.5396947651	2.0291883832	1.4904269075
C	2.6186726087	1.8048752013	-1.1001425322
H	2.4339474201	2.8770652374	-1.2535147822
H	3.7019074479	1.6539925518	-1.0685457973
H	2.216267726	1.2675977102	-1.9638279057
H	2.216267726	1.2675977102	-1.9638279057

TS 6-31++G(d,p) 0096

E(UwB97XD) = -1036.74047781 A.U.

First frequency = -1593.2386 cm^{-1}

S	0.6281025607	-1.4780782095	-0.0440875479
O	1.1051061855	-2.083135698	-1.2908378202
O	-0.3866043814	-2.1893918221	0.7383733588
N	0.0052817413	0.0119424114	-0.4150845927
C	0.9498238167	0.9120597032	-1.0920988645
H	1.2808762228	0.4255312882	-2.0135049651
H	0.3867667689	1.8053986086	-1.3850549244
C	2.1668449682	1.2861843081	-0.2408021587
H	2.3554138048	0.141305622	0.3577566161
C	-1.090961476	0.5692335785	0.3938755984

H	-0.9097461733	1.643918375	0.4710148273
H	-1.0582669885	0.16569337	1.4115926528
C	-2.4555867747	0.2974460606	-0.232955403
H	-2.5527490028	-0.7841359915	-0.3784572509
H	-2.4870350837	0.7597165245	-1.2295324598
C	-3.636612634	0.8042075103	0.6053519505
H	-3.5728848173	0.330215124	1.5955341485
C	-3.6033002598	2.3238084849	0.8016878284
H	-4.4883854976	2.6628722522	1.3498509654
H	-3.5927102368	2.8361690751	-0.1684817612
H	-2.7241661745	2.6510100757	1.3656009337
C	-4.9585507749	0.3760104245	-0.0374198965
H	-5.8126621067	0.6892005617	0.5719725293
H	-5.0077556932	-0.7111402967	-0.1582771572
H	-5.0691544678	0.8306282044	-1.0295631969
C	2.0557337626	-1.094520729	0.9355929056
H	1.7330297991	-0.8227995735	1.9415121863
C	3.2397363715	-2.0171194177	0.8277112288
H	4.0773788803	-1.5918952664	1.3866904476
H	3.5420563468	-2.1458994967	-0.2137672027
H	3.0224454419	-3.0061015889	1.2476010084
C	1.8890434623	2.2472724215	0.896756474
H	1.5639719235	3.2205696294	0.5046164835
H	1.1045792821	1.8766949791	1.5635917957
H	2.7892268583	2.4105523669	1.4965974037
C	3.4053474697	1.5982290495	-1.0496112544
H	3.6390864933	0.7904632531	-1.7501799207
H	3.2611950213	2.5171783364	-1.6352618084
H	4.2705293326	1.7547847071	-0.3987340199
H	4.2705293326	1.7547847071	-0.3987340199

TS 6-31++G(d,p) 0097

E(UwB97XD) = -1036.74116917 A.U.

First frequency = -1510.9147 cm⁻¹

S	0.6404645833	-1.2281352306	1.0323313895
O	-0.36471402	-2.2843943268	0.8821211124
O	1.2867379616	-1.098825215	2.3473852333

N	-0.0924026067	0.2176866843	0.5728250224
C	0.8002675167	1.3811473936	0.7740847462
H	0.2145999866	2.2672942548	0.5065971952
H	1.0809369911	1.4759981148	1.8315479509
C	2.0444454303	1.3136904653	-0.1087927787
H	2.2230775392	0.0363386188	-0.1867269146
C	-1.4662801016	0.3728501871	1.1137117417
H	-1.6090462992	1.4426705612	1.2937729525
H	-1.5454255257	-0.1110016206	2.0940490744
C	-2.5598195638	-0.1492377101	0.1775629933
H	-3.413327451	-0.4457901924	0.7996386206
H	-2.2016534945	-1.0621409168	-0.3104643396
C	-3.0608478653	0.8449290607	-0.878721985
H	-3.4557269321	1.7238930642	-0.34794752
C	-1.9536819195	1.3232608725	-1.819861073
H	-1.4733012401	0.4716278949	-2.3167044124
H	-1.1770934395	1.877434901	-1.2866982091
H	-2.3609130036	1.9831135018	-2.5933913823
C	-4.2098807164	0.2217191564	-1.6761204352
H	-3.8597042355	-0.6566231356	-2.2321697755
H	-4.6202920129	0.9344378551	-2.3990523492
H	-5.0238639286	-0.1004787924	-1.0179852917
C	1.9146926169	-1.3287624752	-0.1788723297
H	2.7814710752	-1.8300888739	0.2499586261
C	1.4871699994	-1.7295903394	-1.5642979902
H	0.6109021021	-1.1604777954	-1.8859682957
H	1.2405545144	-2.7955408169	-1.6105836119
H	2.3023705972	-1.5370112616	-2.266717222
C	3.2868901196	1.887074318	0.5354612499
H	3.1671782482	2.9665613728	0.7022824165
H	3.4850928651	1.4192059887	1.5045916033
H	4.1617307759	1.7465251452	-0.1059097784
C	1.8152934488	1.737243659	-1.5446512144
H	1.6344126768	2.8197888608	-1.5942889442
H	2.6889712993	1.5143991122	-2.1643452517
H	0.946659474	1.2329557572	-1.9753171882
H	0.946659474	1.2329557572	-1.9753171882

TS 6-31++G(d,p) 0103

E(UwB97XD) = -1036.73972866 A.U.

First frequency = -1497.7592 cm⁻¹

S	0.4243065154	-1.4666720241	-0.4565585341
O	1.2115490384	-1.909819042	-1.6173530719
O	-0.7245856012	-2.2966389439	-0.0791074237
N	-0.1510913519	0.093025634	-0.6688871362
C	0.9024681679	1.0442589767	-1.0840622671
H	1.3935027707	0.7070986159	-2.0068119191
H	0.3956036544	1.9897191705	-1.3023898192
C	1.9235602367	1.2645236158	0.0265962276
H	1.9415133127	0.0869538543	0.552870881
C	-1.4342530643	0.1773992544	-1.4047383989
H	-1.5192388164	-0.6283082472	-2.1435317242
H	-1.3917167568	1.1108396128	-1.9723014588
C	-2.6655948005	0.1999030104	-0.5015769821
H	-2.8140906491	-0.7887984825	-0.0554439263
H	-3.5225100663	0.3770985032	-1.1638375668
C	-2.626991736	1.2740378236	0.6046025361
H	-1.935508762	2.0684132415	0.2872187337
C	-4.0070395887	1.9074547897	0.8042950543
H	-4.7438096403	1.1433544146	1.0811323091
H	-4.3574826212	2.3954518189	-0.1114155207
H	-3.9865785993	2.6571574888	1.602675437
C	-2.1116568666	0.7004681236	1.9281819477
H	-2.0040235676	1.4855690934	2.6848751817
H	-1.1427827374	0.2134815532	1.7947094449
H	-2.8129503655	-0.0485010323	2.31583617
C	1.5335246418	-1.2054648417	0.8920693487
H	0.9590202422	-1.0579076723	1.8064721076
C	2.7278538227	-2.1166647544	0.9695363436
H	3.3864562909	-1.7714380113	1.7704291488
H	3.2855895716	-2.1143903454	0.0305219445
H	2.437220974	-3.1491821627	1.1952761223
C	1.4302485665	2.1653911809	1.1391973736
H	1.3865132755	3.2056162173	0.7887966156
H	0.4266253442	1.8764052601	1.4633768165

H	2.1000030457	2.1309421526	2.0037346961
C	3.3257096108	1.5484110236	-0.4620613651
H	3.3569369772	2.5035521143	-1.0044557744
H	4.025421076	1.6209443806	0.3756398531
H	3.6766226603	0.7666961286	-1.1430111502
H	3.6766226603	0.7666961286	-1.1430111502

TS 6-31++G(d,p) 0109

E(UwB97XD) = -1036.74323252 A.U.

First frequency = -1522.6526 cm^{-1}

S	0.5370597521	-1.5732779578	-0.2729888317
O	0.9748497139	-1.7868431727	-1.6607971936
O	-0.4950157089	-2.4788396362	0.2458780226
N	-0.0212825463	-0.010887299	-0.0328251888
C	0.9243883495	1.0209644095	-0.5015956392
H	1.2018085544	0.8433681331	-1.5494584427
H	0.3928961544	1.9777546425	-0.4621419595
C	2.1569449059	1.0763798841	0.3907685482
H	2.3010150483	-0.1877305731	0.6209211842
C	-1.4335770006	0.229553944	-0.3736594994
H	-1.9503328298	-0.7312618273	-0.3681343812
H	-1.5084465722	0.6425768931	-1.3897543032
C	-2.0730722949	1.1721352489	0.6430582781
H	-1.438163863	2.0585520154	0.7671279992
H	-2.1005695899	0.6676030027	1.6178132003
C	-3.4855141449	1.6312253856	0.2575717509
H	-3.4201942508	2.13569705	-0.7172601314
C	-4.4597484588	0.4566058878	0.1214380343
H	-4.1730030287	-0.2279638675	-0.6827097911
H	-5.4704589493	0.8160491657	-0.0974202805
H	-4.5015287211	-0.1178787753	1.0550354277
C	-4.0047661215	2.6456114013	1.279966152
H	-4.9938876746	3.0191646299	0.9958112648
H	-3.3303427295	3.5041003659	1.3673471385
H	-4.0923132236	2.1834763314	2.2708113598
C	1.9694070969	-1.5387501027	0.76209026
H	1.6547359742	-1.6055921271	1.8033019619

C	3.1285807372	-2.3974979486	0.3353684226
H	3.4221106649	-2.1802860986	-0.6939669325
H	2.8926948229	-3.4654829146	0.407951273
H	3.9786341092	-2.1971422032	0.9924251795
C	1.8944683083	1.6795420684	1.7540753682
H	1.7368458712	2.7628650211	1.6627816505
H	0.9991258165	1.2449015149	2.2088433877
H	2.741787294	1.5199689449	2.4274920767
C	3.4119949924	1.55462296	-0.3019856354
H	4.2766096624	1.4887319265	0.3648300751
H	3.6202475786	0.9671808387	-1.2017154525
H	3.3061225212	2.6055363279	-0.6053406948
H	3.3061225212	2.6055363279	-0.6053406948

TS 6-31++G(d,p) 0110

E(UwB97XD) = -1036.74293736 A.U.

First frequency = -1519.1285 cm⁻¹

S	0.5705470022	-1.6144039285	-0.0323680016
O	0.9886604588	-1.9679300207	-1.3975678717
O	-0.4054425664	-2.4996500277	0.6145175497
N	-0.0572351492	-0.0611838788	0.0409873951
C	0.8297584943	0.9509173422	-0.5664276325
H	1.0945814223	0.6663872756	-1.5938706609
H	0.2543918651	1.8809676777	-0.6224123896
C	2.0758899077	1.1642016329	0.2820680859
H	2.2840641591	-0.0563577271	0.6526501276
C	-1.4832123251	0.0721469822	-0.3067898948
H	-1.9640556646	-0.8990659868	-0.169812832
H	-1.5769099145	0.3439838888	-1.3656711203
C	-2.1583245188	1.0967870722	0.6016149626
H	-1.6678242833	2.0750390158	0.499650092
H	-2.0048632632	0.7741026666	1.6379696997
C	-3.660587048	1.2689800076	0.3367533516
H	-4.1310197289	0.2778493458	0.4062390777
C	-4.2812870072	2.1625133499	1.4141168407
H	-3.8390567595	3.1659701504	1.3838846083
H	-4.1164564339	1.7517438479	2.4156840629

H	-5.3606442077	2.2676295675	1.2637276742
C	-3.9453879412	1.8367158232	-1.0577999669
H	-3.4431972372	2.8035179573	-1.1877656411
H	-5.0194987379	1.995768563	-1.1979905322
H	-3.6052543961	1.1699039148	-1.8556215986
C	2.0208861528	-1.3960975573	0.9540636829
H	1.7322551753	-1.3585886907	2.004215746
C	3.2113938329	-2.2428614145	0.5951037887
H	3.0288141459	-3.3059877797	0.7898713629
H	4.0636609986	-1.9324073555	1.2047551764
H	3.473578907	-2.1275300939	-0.4588965419
C	1.8132721215	1.9095991876	1.5731389641
H	0.9478130642	1.4923339912	2.0967938106
H	2.6801405189	1.8657207532	2.2391589674
H	1.6045714499	2.9672349051	1.3619257718
C	3.2925387869	1.613538297	-0.49371558
H	3.1302443764	2.6151757731	-0.9156089734
H	4.1724907208	1.6663796482	0.1538563873
H	3.5106361551	0.9337629451	-1.3233952757
H	3.5106361551	0.9337629451	-1.3233952757

TS 6-31++G(d,p) 0125

E(UwB97XD) = -1036.74258464 A.U.

First frequency = -1517.6986 cm⁻¹

S	0.5770338165	-1.4086837927	-0.9142718217
O	1.3280075961	-1.661903705	-2.1535536605
O	-0.453789345	-2.3877529431	-0.5538079244
N	-0.159684142	0.094785863	-0.9455363147
C	0.7703727103	1.1761669803	-1.3331534818
H	1.2500673115	0.9564878208	-2.2960743609
H	0.1660137105	2.0796226544	-1.4645980576
C	1.8146476284	1.4159808135	-0.2487499709
H	2.0004925631	0.2007296013	0.1489594138
C	-1.5122630279	0.1257865994	-1.5460953522
H	-1.5890352734	-0.5708992743	-2.3893318429
H	-1.6279094478	1.1269392328	-1.9676106258
C	-2.6285976058	-0.1490261479	-0.5378021478

H	-2.6283509098	-1.2136084892	-0.2868867503
H	-3.5805506367	0.0602418211	-1.0460481689
C	-2.5554625457	0.6680634944	0.7577416909
H	-1.6152466158	0.40374782	1.2588989874
C	-2.5497658599	2.1768832046	0.5009586747
H	-2.5463615484	2.7319336816	1.4449329658
H	-3.440790136	2.4778947994	-0.0641129464
H	-1.6688857869	2.4948272294	-0.06538613
C	-3.7106312488	0.2824876201	1.6852247381
H	-4.6757753308	0.5371826909	1.2299794641
H	-3.6416051048	0.8113727771	2.6416595781
H	-3.7105995397	-0.7929859492	1.8921348636
C	1.7402319808	-1.1508496572	0.3889582555
H	1.2099964462	-1.1358779864	1.3410689743
C	3.0175322658	-1.9422917139	0.3207164252
H	2.8410242866	-3.0131631647	0.4745883354
H	3.6917200343	-1.5976751213	1.1088746562
H	3.5102330968	-1.8107449935	-0.6451295402
C	1.2732903133	2.1231975339	0.9755972067
H	0.347887358	1.6539532078	1.322377978
H	1.9996567869	2.1095141167	1.7936384033
H	1.0516430071	3.1728263128	0.7391003017
C	3.1407988852	1.9285855331	-0.7614930494
H	3.0233463621	2.9321417351	-1.1935404795
H	3.872430217	2.0012748285	0.0484120826
H	3.5467447253	1.2757009331	-1.5405309527
H	3.5467447253	1.2757009331	-1.5405309527

TS 6-31++G(d,p) 0126

E(UwB97XD) = -1036.74327741 A.U.

First frequency = -1535.8809 cm⁻¹

S	0.1018140329	-1.0078822016	0.5110588924
O	-0.261118593	-1.54537819	-0.8081294832
O	-0.6728876028	-1.4792527209	1.6652772429
N	0.0559032622	0.6557313302	0.5403305196
C	0.787892189	1.3101325001	-0.5558118961
H	0.4132976491	0.9771983423	-1.5321424373

H	0.5811876672	2.3828825699	-0.4736733389
C	2.290339451	1.0710272871	-0.4361726212
H	2.2846233915	-0.1339701626	0.0393871547
C	-1.1067064117	1.3539644484	1.1095709749
H	-0.7070071146	2.2343213389	1.6253991188
H	-1.5344780894	0.7041462202	1.8745810719
C	-2.1707450007	1.8060520798	0.1060621209
H	-1.7162722889	2.5048214536	-0.6078907832
H	-2.9101902059	2.3916080146	0.6703481263
C	-2.896153338	0.7003503452	-0.6707794695
H	-2.1412096512	0.0875306659	-1.1796775819
C	-3.7082799497	-0.2136142092	0.2513486054
H	-4.4624682601	0.3659536783	0.7989280848
H	-3.0752508937	-0.7273764826	0.9804190067
H	-4.2311449822	-0.9806724572	-0.3293890089
C	-3.796263158	1.3224517123	-1.7420142086
H	-4.5686282616	1.951597912	-1.2820752525
H	-4.301060999	0.5480463157	-2.3288236548
H	-3.2201440069	1.9479478707	-2.4325706749
C	1.8374131961	-1.2643309903	0.7242166626
H	2.1035719591	-1.0441965855	1.7580024814
C	2.4218837463	-2.508103611	0.112672458
H	2.1774849664	-2.5768921755	-0.9495314271
H	2.0576746316	-3.4150969585	0.6091522062
H	3.5091129487	-2.4807636289	0.2217946232
C	2.9463418234	1.8861728062	0.657926839
H	2.9982225791	2.9429806789	0.3630383641
H	2.375068364	1.8221436777	1.5894553297
H	3.9665501999	1.5415640023	0.8516804078
C	3.0286426379	1.0364860073	-1.7540409066
H	2.5854454448	0.3080682597	-2.4403119481
H	2.9917422338	2.0208797202	-2.2412559433
H	4.0819375765	0.7804175338	-1.6067695156
H	4.0819375765	0.7804175338	-1.6067695156

TS 6-31++G(d,p) 0127

$E(U_wB97XD) = -1036.73352616$ A.U.

First frequency = -1537.8788 cm^{-1}

S	0.2990002893	-1.2890499874	0.4061417014
O	0.1435146421	-1.6814044704	-1.0000835858
O	-0.3988671107	-2.1334673551	1.3862634163
N	-0.2171389593	0.2736541116	0.6301059731
C	0.6724378919	1.4375569837	0.4645682004
H	0.0846325599	2.231578556	-0.0134210429
H	0.9494259433	1.793803823	1.4673329168
C	1.9338505316	1.2048892682	-0.3526344657
H	2.2485174112	0.0268470565	0.0872793034
C	-1.3906484451	0.5215437817	1.4754533119
H	-1.0502783798	0.9563237214	2.4268421152
H	-1.8455241029	-0.4398639266	1.7117271521
C	-2.4338739297	1.4532787011	0.8526758477
H	-2.014390741	2.4584641669	0.7215271539
H	-3.2185424176	1.5559877348	1.6133121439
C	-3.0883415553	1.0027914184	-0.4671224618
H	-3.9632423548	1.6543901831	-0.5968950246
C	-2.1898307249	1.2112206829	-1.6919078284
H	-1.8218794059	2.2424854055	-1.7416988232
H	-2.7479371872	1.0113077615	-2.6131203915
H	-1.3275504999	0.5401749459	-1.6670889996
C	-3.5984419174	-0.4398308744	-0.4005664224
H	-2.7698224243	-1.1555336825	-0.3645777697
H	-4.1963654417	-0.6769081285	-1.2865067596
H	-4.2252549033	-0.6022735957	0.4835492391
C	2.0303985955	-1.1815260209	0.7344106701
H	2.1848040483	-0.9509586291	1.7892843781
C	2.8936407096	-2.2554532131	0.1296349486
H	3.9432401433	-2.0166275971	0.318265061
H	2.7375133683	-2.322650362	-0.9491755954
H	2.6871522974	-3.2374775379	0.570725622
C	3.0686737478	2.1212314969	0.053433216
H	3.9738087044	1.8944672581	-0.5168261174
H	2.8039910976	3.1689274603	-0.1457189396
H	3.2977602641	2.0316219217	1.1198964373
C	1.7273938367	1.0886333154	-1.8489675352
H	2.6594271652	0.8064030665	-2.3474194544
H	0.9642469358	0.3490666173	-2.099323499

H 1.4099315455 2.0595309775 -2.2537264664
H 1.4099315455 2.0595309775 -2.2537264664

TS 6-311++G(d,p) 0001

E(UwB97XD) = -1036.89146866 A.U.

First frequency = -1553.3273 cm⁻¹

S 0.2654741818 -1.2260392043 0.2989891804
O -0.3786087137 -2.2918181781 -0.4643396738
O -0.1823223325 -1.0125260462 1.6762222004
N 0.1431688694 0.1616753961 -0.6093963746
C 0.7236138161 1.3552049447 0.0218822322
H 0.4877557972 2.2015854891 -0.6303027734
H 0.2566725287 1.5498805016 0.9940720444
C 2.2363257816 1.2282816885 0.1608365761
H 2.333006944 -0.0452008498 0.3989686111
C -0.9842949364 0.3471746189 -1.5329545695
H -1.3056758228 -0.6419793236 -1.8581955593
H -0.5763907195 0.8536841832 -2.4133717327
C -2.1593431215 1.1612790611 -0.9900223777
H -2.868662808 1.2880531775 -1.8182008977
H -1.8102224968 2.1692219032 -0.7377207192
C -2.8981619979 0.5731879198 0.2163724332
H -2.1649714437 0.3896148147 1.0099994316
C -3.9174973568 1.5837245129 0.7446507802
H -3.4357851 2.5249036507 1.0264734146
H -4.437114743 1.1938150863 1.6244986055
H -4.672171947 1.8074780428 -0.0180265024
C -3.5797176718 -0.7548934297 -0.1179612813
H -4.1148756953 -1.1430973153 0.7533994774
H -2.8622221359 -1.5171990828 -0.4297168397
H -4.3083284479 -0.6186878667 -0.9257581811
C 2.0191760131 -1.4070242896 0.3576649108
H 2.3073881925 -1.8114286807 1.3251230034
C 2.667832533 -1.9914482025 -0.8652525176
H 2.3074365951 -1.5056020878 -1.7742686385
H 2.4685946671 -3.0638829439 -0.9476131346
H 3.7493532852 -1.8505642873 -0.8067932679

C	2.818299954	1.9459319996	1.3541967531
H	2.3319873095	1.6349615466	2.282520861
H	3.8908154544	1.7559878591	1.4419045783
H	2.6816428383	3.0304904189	1.2522966653
C	2.9789002516	1.4304333591	-1.1406291533
H	2.5011254731	0.8829316742	-1.9567420237
H	2.9833113717	2.4951525665	-1.4068551415
H	4.018372162	1.101711546	-1.0630052782
H	4.018372162	1.101711546	-1.0630052782

6311Gdp TS-relax-1-5-0004

E(UwB97XD) = -1036.89116048 A.U.

First frequency = -1548.4409 cm⁻¹

S	0.5599080186	-1.1891283902	0.6886826278
O	-0.16681111	-2.3383795659	0.1556219891
O	0.3301548169	-0.8379560866	2.0916094114
N	0.2348570113	0.0966943228	-0.3293348197
C	0.8649946822	1.3562056938	0.1028329007
H	0.4639269833	2.1431169449	-0.5442688623
H	0.5893536027	1.6040280657	1.1339113562
C	2.3789788892	1.2814010511	-0.0446129397
H	2.5675768697	0.0422144945	0.2946245498
C	-1.1315949995	0.1879861345	-0.8603371114
H	-1.3912349131	-0.7952330456	-1.2517825021
H	-1.073616262	0.8706978396	-1.7141135755
C	-2.1808547629	0.6775145903	0.1363387092
H	-1.8327547449	1.6108833077	0.5927365967
H	-2.2782580153	-0.0523055634	0.949532143
C	-3.557065369	0.9197500283	-0.4940245179
H	-3.4276483918	1.636089096	-1.3165854648
C	-4.1631660591	-0.3626375132	-1.069401167
H	-5.1649332319	-0.1726216493	-1.4648798945
H	-4.2487806558	-1.128268535	-0.2902991761
H	-3.5621615333	-0.7773156665	-1.8825480346
C	-4.5024919458	1.5455068672	0.5322217514
H	-4.6617772703	0.8626332131	1.3740114538
H	-5.4780400016	1.7622364652	0.0877974196

H	-4.0958310142	2.4797618152	0.9301815284
C	2.3036474723	-1.3232766404	0.4612727996
H	2.7664709589	-1.6040313749	1.4044930006
C	2.7610076309	-2.0336143895	-0.7814562767
H	3.8341177717	-1.8798106513	-0.913830577
H	2.2475137012	-1.6522343825	-1.6662610735
H	2.577435599	-3.1100192138	-0.7155946337
C	3.1460091741	2.127949868	0.941958273
H	2.8587165609	1.9001831491	1.9717926954
H	4.2226487062	1.97291939	0.8379994726
H	2.9466420198	3.1932610872	0.7671627416
C	2.8556737027	1.3670113642	-1.476679201
H	2.7642508064	2.3987956996	-1.839515531
H	3.9049755064	1.0744384908	-1.5656495209
H	2.2584009917	0.7269451553	-2.1301721914
H	2.2584009917	0.7269451553	-2.1301721914

TS 6-311++G(d,p) 0007

E(UwB97XD) = -1036.89104673 A.U.

First frequency = -1547.4913 cm^{-1}

S	0.5991415499	-1.2682281779	0.6719240436
O	-0.0871951503	-2.4539439993	0.165685866
O	0.3814128658	-0.9116929173	2.0754257148
N	0.1997319518	-0.0099093007	-0.3545570377
C	0.7781997397	1.2822880769	0.0537456691
H	0.3374747992	2.0408207502	-0.6014442818
H	0.4988036457	1.5326147562	1.0832496298
C	2.2927529566	1.273615473	-0.1065551332
H	2.5410922989	0.0466011615	0.2366275426
C	-1.1796893209	0.0205454288	-0.8588771295
H	-1.4188282954	-0.9771710094	-1.2311968481
H	-1.1554266398	0.6895854311	-1.7224391077
C	-2.2290448741	0.471492015	0.1561208368
H	-1.9930617064	1.4834204816	0.5096459684
H	-2.1766280904	-0.1863629827	1.0302188036
C	-3.6599260609	0.4558295763	-0.394257161
H	-3.8641961416	-0.5568955606	-0.7661726788

C	-4.6559547748	0.7567204308	0.7264675617
H	-4.5553369652	0.0433399782	1.5493263428
H	-5.6856458649	0.7102150552	0.3607488132
H	-4.4886066426	1.7616650333	1.1299302386
C	-3.846912746	1.4371525892	-1.5539667573
H	-3.2253998634	1.1847742385	-2.4168177555
H	-3.5910425709	2.4553172191	-1.2391400897
H	-4.8873947255	1.4429695912	-1.8906037826
C	2.3422824231	-1.328645366	0.4131528617
H	2.83328856	-1.5835302309	1.3494749695
C	2.8091793945	-2.0237440691	-0.8345868541
H	2.6773230638	-3.1071690072	-0.7602955894
H	3.8714454431	-1.8210599163	-0.9874414413
H	2.2623194668	-1.6710786999	-1.711306652
C	3.0305980572	2.1584045028	0.8686861278
H	2.7630635054	1.9231258009	1.9021484402
H	4.1120254087	2.0503969147	0.7553756523
H	2.7828522675	3.2130131484	0.6910419162
C	2.752163787	1.3719368416	-1.5435078792
H	2.1799259666	0.7000156691	-2.1874212246
H	2.6090704346	2.3957556021	-1.9121097141
H	3.8131939893	1.1282416143	-1.6403664363
H	3.8131939893	1.1282416143	-1.6403664363

TS 6-311++G(d,p) 0016

E(UwB97XD) = -1036.89005142 A.U.

First frequency = -1539.0027 cm⁻¹

S	0.6029842039	-1.3330646875	0.327138328
O	0.438295051	-1.8642996296	-1.0277572713
O	-0.0938876159	-2.0344470339	1.4031295045
N	0.1491874162	0.2711959557	0.4274475919
C	0.7477420143	1.1202179754	-0.617815925
H	0.5372634972	0.7236779	-1.6174940593
H	0.259011316	2.0969287999	-0.5420912675
C	2.2474948202	1.2680448443	-0.4004693155
H	2.5171236366	0.0783849415	0.0321592623
C	-1.2548550408	0.541480914	0.7664577226

H	-1.274664263	1.5814994593	1.101077733
H	-1.5138797245	-0.078233451	1.6267172448
C	-2.2491984999	0.3108570827	-0.3704978405
H	-2.1548449909	-0.7246902613	-0.7141672201
H	-1.9913158119	0.950241304	-1.2245583152
C	-3.706513951	0.5732714466	0.0270519329
H	-3.9331042948	-0.052519511	0.9003735095
C	-3.9499727309	2.0349810312	0.4105954755
H	-3.6769443803	2.6987394819	-0.4177213894
H	-3.3731407513	2.3367713923	1.2884512786
H	-5.0060700487	2.2031327498	0.6393860886
C	-4.642369723	0.1557540327	-1.1080864238
H	-4.5025064541	-0.8965198848	-1.3713028869
H	-4.450243681	0.75537876	-2.0048951256
H	-5.6896883459	0.2993485388	-0.8276306085
C	2.3330221852	-1.1700495137	0.6360006632
H	2.4860313977	-0.9568676185	1.6920414223
C	3.2297780237	-2.1910616089	-0.0044920476
H	3.0455756103	-2.2567085737	-1.0777866201
H	3.0877186015	-3.1861940816	0.4300940488
H	4.2707162278	-1.9028512015	0.1555975301
C	2.6091249475	2.1686152127	0.7585726437
H	3.6706282565	2.0886682057	1.0062677979
H	2.4023829237	3.2152964389	0.5020733593
H	2.0245934144	1.9163001521	1.6469855534
C	3.04594073	1.4805333795	-1.6633804541
H	2.7898215522	2.4448339681	-2.1216398139
H	4.1180974831	1.4909093887	-1.4526025678
H	2.8433185773	0.698522051	-2.4000254608
H	2.8433185773	0.698522051	-2.4000254608

TS 6-311++G(d,p) 0017

E(UwB97XD) = -1036.89046547 A.U.

First frequency = -1544.8507 cm^{-1}

S	0.2867532672	-1.0092824073	0.6737206939
O	-0.0853921824	-1.7629581443	-0.524833283
O	-0.396439527	-1.3562313255	1.9183319376

N	0.1038678848	0.6273653749	0.4586109383
C	0.7358772627	1.1640678915	-0.7550616456
H	0.35758935	0.6574202239	-1.650261369
H	0.4398060181	2.2151197917	-0.8249028953
C	2.2543346035	1.0664737509	-0.6745316103
H	2.3662451196	-0.0558400976	-0.0379867886
C	-1.0825488765	1.3166664734	0.9843850468
H	-0.7338397234	2.2892945832	1.3454355391
H	-1.4243752693	0.7600010227	1.8565810019
C	-2.2196596116	1.5345876367	-0.0143800531
H	-1.8549385505	2.1515341419	-0.8437890866
H	-2.9804855181	2.1386696366	0.4968935796
C	-2.8804325842	0.274860829	-0.5829943561
H	-2.0997350308	-0.3450066561	-1.0382775559
C	-3.5711090439	-0.5521196912	0.5028584616
H	-2.8672908494	-0.9017946153	1.2615177361
H	-4.0516931992	-1.433353311	0.0683347218
H	-4.3465106748	0.041300407	1.0014541305
C	-3.8733650372	0.6596337227	-1.680848145
H	-3.3826531121	1.2185769152	-2.4833918594
H	-4.675057681	1.2874552713	-1.2753789277
H	-4.3350379433	-0.228558135	-2.1214472699
C	2.0429332586	-1.1014469924	0.8291328067
H	2.3309789699	-0.70598339	1.8013259603
C	2.6977094669	-2.3760542292	0.3780704772
H	2.4101996217	-2.6254537925	-0.6442848559
H	2.4331202791	-3.2193796086	1.0247462343
H	3.782128981	-2.2538780186	0.4170813778
C	2.8738918901	2.0754981782	0.2654411593
H	2.8194643761	3.0810841291	-0.1702473766
H	2.3459783353	2.0931237412	1.2227174304
H	3.9263660603	1.8487535553	0.4536812681
C	2.9450217611	0.9065927276	-2.0065104068
H	2.5411360354	0.0585252939	-2.5659030074
H	2.8083995001	1.8065657871	-2.620460179
H	4.019666937	0.7575592526	-1.8759390951
H	4.019666937	0.7575592526	-1.8759390951

TS 6-311++G(d,p) 0018

E(UwB97XD) = -1036.89209774 A.U.

First frequency = -1547.4463 cm⁻¹

S	0.4406563481	-1.5003299635	-0.3037673829
O	1.236191807	-2.0767066596	-1.390094177
O	-0.7051649323	-2.2792747679	0.1611315906
N	-0.1244856032	0.0161888274	-0.6905579143
C	0.9160031278	0.9352237817	-1.1792812588
H	1.4591475198	0.4906174372	-2.0218312426
H	0.4021248467	1.8249494748	-1.5546209292
C	1.8694927908	1.3217629149	-0.0584073749
H	1.9262117453	0.1863835492	0.5615503879
C	-1.4444296531	0.1217462248	-1.3283944169
H	-1.961222344	-0.830244778	-1.2101882294
H	-1.3207849257	0.2941668471	-2.4033149327
C	-2.255721366	1.2472828685	-0.6925919454
H	-3.1786593912	1.373561095	-1.2720220704
H	-1.7007429159	2.187908882	-0.7923251326
C	-2.603499311	1.0214373572	0.7830548056
H	-1.6748826426	0.7574348634	1.3034084215
C	-3.1459761786	2.3094410447	1.4022806495
H	-3.3819472476	2.1688330311	2.4609737231
H	-4.0637510402	2.6270143017	0.8944548649
H	-2.4196696924	3.1241769424	1.3227491806
C	-3.5910438134	-0.131527287	0.9692990929
H	-4.528255451	0.0742419023	0.4395622442
H	-3.8284280073	-0.2690779044	2.028161391
H	-3.1866804349	-1.076120483	0.5980241047
C	1.5377501912	-1.0788621881	1.0144507158
H	0.9476596713	-0.8470868407	1.8991054206
C	2.7428929092	-1.9572760743	1.1954041958
H	3.3029189645	-2.051921694	0.2639126194
H	2.4665217684	-2.9615129283	1.5335852427
H	3.3948167357	-1.5179879605	1.9532549713
C	1.2647693288	2.2706322679	0.9511419878
H	0.2767693434	1.9279198515	1.2686422688
H	1.9002083594	2.3683785572	1.8349243242

H	1.1497749632	3.268132614	0.5082779421
C	3.268274509	1.6597942687	-0.5127407853
H	3.9250909405	1.8420126958	0.3412836115
H	3.6970003216	0.8554048047	-1.116417649
H	3.2626949258	2.5704861043	-1.1259433333
H	3.2626949258	2.5704861043	-1.1259433333

TS 6-311++G(d,p) 0019

E(UwB97XD) = -1036.89019197 A.U.

First frequency = -1541.8080 cm^{-1}

S	0.5423842586	-1.3147848281	0.0345067985
O	0.3613608929	-1.5953104612	-1.3914516259
O	-0.2109162819	-2.1426318876	0.973832705
N	0.1889640793	0.2750140877	0.4044845412
C	0.8570673663	1.248118761	-0.4774980828
H	0.6444074081	1.0387607126	-1.5318271786
H	0.4271014702	2.2273048707	-0.2431575536
C	2.3584996242	1.2623611254	-0.2248037496
H	2.5468965491	0.0009856321	-0.0045576374
C	-1.2002458794	0.5685829895	0.7824069225
H	-1.1731744121	1.5438684043	1.2787674449
H	-1.4925304415	-0.1656352027	1.5326654188
C	-2.1944420976	0.5948610196	-0.377395728
H	-2.2662697027	-0.4070682189	-0.8181756054
H	-1.8112741141	1.2562759216	-1.162536291
C	-3.5941431563	1.0702200781	0.0287807537
H	-3.4917292539	2.0645590886	0.4840488812
C	-4.4821938455	1.2070452749	-1.2086231877
H	-4.6129365894	0.2350030614	-1.6967991958
H	-4.0437941445	1.8932276252	-1.9390491032
H	-5.4737122148	1.5837377318	-0.9418614959
C	-4.2448030492	0.1401969968	1.0557474601
H	-3.6874804781	0.1043872761	1.9951719786
H	-4.3065975382	-0.8805137225	0.6622162587
H	-5.2604651439	0.4722491438	1.2885842857
C	2.2750617067	-1.3185682435	0.3715229693
H	2.4256779242	-1.3014475181	1.4490725097

C	3.1158299813	-2.2692932239	-0.4322956197
H	2.9474114913	-2.1347565384	-1.5017081963
H	2.9028170726	-3.3132943606	-0.1794887961
H	4.1700106608	-2.0828287542	-0.2174816317
C	2.7516678768	1.9237165029	1.076413637
H	3.8014925348	1.7353958628	1.3150908455
H	2.613693057	3.0099462182	1.0046374275
H	2.1359945546	1.5583691019	1.9022838956
C	3.1919038176	1.6403911636	-1.424832614
H	4.2585954439	1.5480733232	-1.206521222
H	2.9573179184	1.0114927511	-2.2878076873
H	3.0018488502	2.6832945138	-1.7106443113
H	3.0018488502	2.6832945138	-1.7106443113

TS 6-311++G(d,p) 0029

E(UwB97XD) = -1036.89086794 A.U.

First frequency = -1541.1530 cm⁻¹

S	0.7756639632	-1.4943793505	0.6488631915
O	-0.0801037364	-2.5329915481	0.08117866
O	1.1221196534	-1.6112463627	2.0668953526
N	0.0448627413	-0.0270520915	0.3137780748
C	0.7877221118	1.124719474	0.854616372
H	0.1507705382	2.0040400691	0.7214246924
H	0.9570720657	1.0025729367	1.9312816536
C	2.1011552211	1.3235084337	0.1134477879
H	2.433439644	0.0825626773	-0.0639802884
C	-1.4164258111	0.0346397525	0.4589367493
H	-1.6785665312	0.4499197905	1.4410267088
H	-1.8029586437	-0.9831814026	0.4180896023
C	-2.027837767	0.8693382457	-0.6612933549
H	-1.8466179148	0.3592603695	-1.6151932073
H	-1.5108822194	1.8339403323	-0.7192304964
C	-3.5289208131	1.1268995925	-0.4902647789
H	-3.6744443651	1.6332904628	0.4732249296
C	-4.0300355507	2.0593697442	-1.5937962823
H	-5.091137155	2.289286733	-1.4627090504
H	-3.9074561509	1.5920784921	-2.5771842885

H	-3.4769476812	3.0031930982	-1.5989444505
C	-4.339322868	-0.1712111308	-0.4732200645
H	-4.1687434945	-0.7415841822	-1.3932112415
H	-5.409678319	0.0421632638	-0.4044681913
H	-4.0769714947	-0.81176119	0.3726759466
C	2.2784863203	-1.2970596503	-0.2531537296
H	3.0891712347	-1.768861729	0.2972268612
C	2.2000190337	-1.544199266	-1.7334452323
H	2.0691842932	-2.6076755321	-1.9534259871
H	3.1259118395	-1.2104242785	-2.2067502854
H	1.3680764211	-0.9968602536	-2.1811563055
C	3.1955625107	1.9579591138	0.936806499
H	2.9220784631	2.9858143535	1.2084935842
H	3.3706403104	1.4042304098	1.8629472559
H	4.1320784702	2.003532833	0.3757608012
C	1.9294362836	1.8866660889	-1.2789885942
H	1.122590489	1.3789087888	-1.812656435
H	1.6757941242	2.9529845713	-1.220862859
H	2.8484347605	1.7941467463	-1.8632409452
H	2.8484347605	1.7941467463	-1.8632409452

TS 6-311++G(d,p) 0031

E(UwB97XD) = -1036.89062569 A.U.

First frequency = -1535.3864 cm⁻¹

S	0.8018290132	-1.4486099318	0.8558360263
O	0.0106580994	-2.5950521377	0.4163578835
O	1.0932622999	-1.3443859407	2.2873000976
N	0.0289141182	-0.0791279873	0.2844188085
C	0.7080061477	1.170295814	0.6709947442
H	0.0411908135	1.9919447853	0.3940650151
H	0.8474133617	1.2129675747	1.7580589331
C	2.0358092439	1.316329163	-0.0561030825
H	2.4251692716	0.0796361785	-0.0305550729
C	-1.4380935	-0.0559510815	0.3887436972
H	-1.7312538079	0.4783173204	1.2993830742
H	-1.7942279084	-1.0830746104	0.4795712497
C	-2.0486860672	0.5765737082	-0.8573497617

H	-1.7113797707	-0.0024312282	-1.7234261235
H	-1.6631897712	1.5957207915	-0.9910179165
C	-3.5809445707	0.6270445457	-0.8412833311
H	-3.9492442481	-0.3909819701	-0.6585191332
C	-4.1204412863	1.5367452033	0.2653166321
H	-3.8482138517	1.184363945	1.2631975403
H	-5.211885198	1.5907663258	0.2226749805
H	-3.7300080863	2.5541182568	0.1481794069
C	-4.1026356881	1.0799557695	-2.2056837583
H	-5.1960367588	1.089826867	-2.2250420866
H	-3.7551457855	0.4180660256	-3.0040634045
H	-3.7545738576	2.0938247748	-2.4331410599
C	2.3321919839	-1.3182728797	-0.0118369461
H	3.1373316734	-1.6632240653	0.6327509921
C	2.3278821443	-1.7883691431	-1.4392475749
H	1.4920079229	-1.3578028912	-1.9942468218
H	2.2552594324	-2.8780796669	-1.4999272044
H	3.2570702678	-1.4820972171	-1.924627461
C	3.072885655	2.1202673661	0.6897541075
H	2.7464428485	3.1634298154	0.7917173554
H	3.2387126471	1.7236175332	1.6948220373
H	4.0257219323	2.1238667626	0.1549767678
C	1.8877849985	1.6519074266	-1.5227747712
H	1.5861277043	2.7011053127	-1.6362660583
H	2.8294349663	1.515857744	-2.0605975371
H	1.1225561022	1.0304016454	-1.9936557376
H	1.1225561022	1.0304016454	-1.9936557376

TS 6-311++G(d,p) 0039

E(UwB97XD) = -1036.88982950 A.U.

First frequency = -1529.4042 cm⁻¹

S	0.6750080661	-1.5452588776	0.2072668162
O	1.0273929578	-2.2885423897	-1.004485046
O	-0.2158564766	-2.2121401238	1.1544816439
N	-0.0184855325	-0.0669636378	-0.1536618288
C	0.7773406488	0.733046955	-1.1020048681
H	0.9964792821	0.1527124214	-2.0067175021

H	0.1549773748	1.5810643802	-1.4019488726
C	2.0565898542	1.2339251893	-0.4504716295
H	2.3484415673	0.1900979698	0.2535751037
C	-1.4698437956	-0.0684089005	-0.3922035401
H	-1.8870794061	-0.9634775004	0.0682785881
H	-1.6721186701	-0.1246743909	-1.4699652369
C	-2.110525507	1.1759387327	0.2134713077
H	-1.5632105741	2.0652122471	-0.1191717095
H	-2.0000002465	1.1304800091	1.3036191235
C	-3.5897510756	1.34694159	-0.1489401769
H	-3.6639539215	1.3877640795	-1.243811491
C	-4.4443306043	0.1765107458	0.3429449215
H	-4.345273597	0.059057738	1.4279401812
H	-4.1592494427	-0.7693230799	-0.1248574564
H	-5.5008807635	0.3486353956	0.1193559884
C	-4.1165572114	2.6694686809	0.4094496834
H	-5.159778727	2.8295934798	0.1230787612
H	-3.5305985946	3.5176323388	0.0433910813
H	-4.0653057641	2.6723435866	1.5038844419
C	2.1678919653	-0.9960832797	0.9736530268
H	1.9371406913	-0.6384613233	1.9751346725
C	3.3691371266	-1.8841324919	0.8134981679
H	3.2475177952	-2.8327787777	1.3468151774
H	4.2436907108	-1.3785732395	1.2278884007
H	3.5580402884	-2.1046206413	-0.2381173046
C	1.8299283959	2.3245207029	0.5714292143
H	1.0231784487	2.0555422396	1.2579526957
H	2.7347633164	2.5168956376	1.1533455366
H	1.5492981	3.2588773834	0.068874139
C	3.1989171122	1.4656451912	-1.4089804826
H	4.1110782612	1.7390911004	-0.8731110425
H	3.4019243467	0.5756563086	-2.0106673998
H	2.9609872264	2.2868638886	-2.0977430212
H	2.9609872264	2.2868638886	-2.0977430212

TS 6-311++G(d,p) 0040

E(UwB97XD) = -1036.89059490 A.U.

First frequency = -1521.0686 cm^{-1}

S	0.4423400544	-1.1820460572	0.9544107502
O	-0.6128342682	-2.1347847104	0.6176770559
O	0.9308780624	-1.1855620138	2.3354072071
N	-0.1148271141	0.3344695987	0.5030881937
C	0.8524186887	1.4081849288	0.7988946947
H	0.3407003564	2.3545850535	0.6004552679
H	1.1215900191	1.3987624863	1.8626462257
C	2.0895823627	1.3031929987	-0.0786866804
H	2.2153605039	0.015980928	-0.1222697285
C	-1.4974317091	0.645361084	0.9149264354
H	-1.4740039633	1.1694455703	1.8776395301
H	-2.0260412633	-0.2945150817	1.075166343
C	-2.2288160624	1.4920524333	-0.1300086189
H	-1.5291836668	2.2197972416	-0.5561684163
H	-2.9925398412	2.0764898877	0.3944826886
C	-2.9157379139	0.7245672311	-1.2721330356
H	-3.345743475	1.492235062	-1.9274480371
C	-1.9467906934	-0.1094593646	-2.1112059627
H	-2.4636323252	-0.5405197786	-2.9739056466
H	-1.5281181002	-0.9309021192	-1.524384724
H	-1.1176935583	0.4993077589	-2.483085225
C	-4.072817057	-0.140574769	-0.766254629
H	-4.6196004464	-0.5798271499	-1.605435196
H	-4.7798886577	0.4465231289	-0.1725241112
H	-3.7140019884	-0.9679408033	-0.1456576627
C	1.8418726199	-1.3328175493	-0.1077874702
H	2.6328697916	-1.8545446689	0.4259591623
C	1.5662273187	-1.7436046	-1.5264070501
H	1.2341438703	-2.784400055	-1.5829852371
H	2.4809421788	-1.6459818386	-2.1149036699
H	0.7971510472	-1.1148983989	-1.9780679585
C	3.3494368408	1.8440898478	0.5531542011
H	4.2152932707	1.6748122087	-0.0914550181
H	3.2619111299	2.9266283475	0.7128422323
H	3.5408668122	1.3787503072	1.5236186501
C	1.8536402655	1.7229825911	-1.5114269264
H	2.6826977617	1.4234507801	-2.1574029042
H	0.9313237496	1.2871951398	-1.9011365024

H 1.7605377531 2.8149601566 -1.5696966671
H 1.7605377531 2.8149601566 -1.5696966671

TS 6-311++G(d,p) 0041

E(UwB97XD) = -1036.88955427 A.U.

First frequency = -1526.1596 cm⁻¹

S 0.7237038842 -1.5886741772 0.2088969318
O 1.0386432565 -2.2924318446 -1.0364827105
O -0.0955239776 -2.3068295161 1.1829928247
N -0.0354942701 -0.127111178 -0.0814432808
C 0.6869921043 0.7220418316 -1.0461514903
H 0.8820732169 0.1712255854 -1.9746321987
H 0.0225743526 1.5545836415 -1.2943199555
C 1.9783291184 1.2519563667 -0.4435812329
H 2.3392702631 0.2025287065 0.2184562119
C -1.4951694528 -0.178122073 -0.2642824562
H -1.8697151639 -1.0924903794 0.1983066481
H -1.7276860606 -0.2285676993 -1.3339450216
C -2.1562016965 1.024667119 0.4005271156
H -1.7583113086 1.9563414436 -0.0221357808
H -1.8758182714 1.015517237 1.458841109
C -3.6843145609 1.0405520021 0.2768397266
H -4.0627813168 0.0829049644 0.65773964
C -4.2662512476 2.1570025543 1.1450736233
H -3.9095648093 3.1352026501 0.8034370881
H -3.9740071281 2.0395552592 2.1924721013
H -5.3587609472 2.1640233315 1.0964224223
C -4.1481306689 1.1953656115 -1.1736369114
H -5.2391397687 1.24904773 -1.2264113662
H -3.8298096225 0.3609537646 -1.8032707873
H -3.7460869075 2.118201747 -1.6071584447
C 2.2344702275 -1.0070141352 0.9139881872
H 2.0434083265 -0.6831998835 1.9351120111
C 3.4550478015 -1.8481989156 0.6693093946
H 4.3318128218 -1.32447327 1.0554721819
H 3.5987963392 -2.032527392 -0.3963457925
H 3.391585074 -2.8151121007 1.1794201847

C	1.7648543115	2.3088203406	0.6159588911
H	2.6898979149	2.5184743525	1.1588765997
H	1.428692262	3.2447383425	0.1518855912
H	1.0018796865	1.9949274016	1.3327808823
C	3.0637623105	1.5466270196	-1.4498379122
H	3.2684534974	0.6782994024	-2.0818672167
H	2.7636073105	2.3736771223	-2.1065511474
H	3.9907164431	1.84116389	-0.9519488273
H	3.9907164431	1.84116389	-0.9519488273

TS 6-311++G(d,p) 0045

E(UwB97XD) = -1036.88920952 A.U.

First frequency = -1503.7042 cm⁻¹

S	0.2190890898	-1.3783203196	-0.3711629106
O	0.854939836	-1.9324907358	-1.5690367637
O	-0.978094491	-2.061474141	0.1152765144
N	-0.190679787	0.2325789313	-0.5739454029
C	0.9252245741	1.0617571555	-1.0683545196
H	1.3021898634	0.6640012017	-2.0192934769
H	0.5076082632	2.0526202409	-1.2705806575
C	2.0448241564	1.177838798	-0.0451739652
H	1.9852983043	0.0022723706	0.4797259155
C	-1.4649479562	0.4666273447	-1.2813895352
H	-2.05876425	-0.4463598136	-1.2392847241
H	-1.2525008026	0.6611040965	-2.3394564255
C	-2.2618744117	1.6300398262	-0.6940648293
H	-3.0129866996	1.8976477718	-1.4461997257
H	-1.6111026779	2.5063262396	-0.5906931173
C	-2.9917590241	1.3793781733	0.6382857463
H	-3.6362834174	2.2553856798	0.7840734122
C	-3.8992091147	0.1482373593	0.5806152991
H	-4.5468651196	0.1694899675	-0.3017239426
H	-4.5392999091	0.103519249	1.4662973184
H	-3.3115105651	-0.7741215574	0.5514821515
C	-2.0556946091	1.3070302425	1.8462169706
H	-1.4414832199	2.2091560667	1.9212865261
H	-1.3869284021	0.4463229954	1.7764448197

H	-2.633599726	1.2165310538	2.7710444126
C	1.4462819821	-1.2229000085	0.8852763312
H	0.9591325094	-0.9788735597	1.8273624129
C	2.5165292962	-2.2768505871	0.9084774585
H	2.9946474834	-2.3720996355	-0.0675246872
H	2.1162710221	-3.2557801723	1.1925578068
H	3.2740635673	-1.9999988126	1.6443551009
C	1.7290034079	2.1054185006	1.10554803
H	0.7530337232	1.8727500463	1.5361172379
H	2.4843922541	2.0314070231	1.8919097647
H	1.7065350932	3.1458287909	0.757456643
C	3.4213094441	1.3325431887	-0.6455891027
H	4.1901686089	1.3280557958	0.1307644874
H	3.6391049044	0.5311097093	-1.3565387125
H	3.4997999075	2.2862686049	-1.1837499768
H	3.4997999075	2.2862686049	-1.1837499768

TS 6-311++G(d,p) 0046

E(UwB97XD) = -1036.89069699 A.U.

First frequency = -1548.2866 cm^{-1}

S	0.4210068585	-1.3409383298	0.3531049732
O	-0.022149336	-2.4890678949	-0.4334116202
O	-0.0655473427	-1.2363271432	1.7300690486
N	0.0354619555	0.016955622	-0.5271773809
C	0.431325582	1.2800362781	0.1147721175
H	-0.0127624091	2.0887439576	-0.471980226
H	0.0308610193	1.3528895357	1.1315067345
C	1.9473597099	1.4255800349	0.1363243919
H	2.266378973	0.1929458396	0.3952457676
C	-1.1683068893	-0.0341674449	-1.3706339971
H	-1.0374360573	-0.8593428219	-2.0722732514
H	-1.1489313393	0.8852528613	-1.9602586825
C	-2.5074207092	-0.2054257056	-0.6518727779
H	-2.4976307148	-1.1693216601	-0.1320249438
H	-3.2806283931	-0.2851997643	-1.4276361525
C	-2.9125397011	0.8929353079	0.3377726684
H	-2.1183378855	0.9906538345	1.0860994243

C	-3.1094472919	2.2467676414	-0.346044405
H	-3.3992176949	3.0106379448	0.3808606769
H	-3.9030133452	2.1821063926	-1.0990147629
H	-2.2047165462	2.5987510302	-0.8482551627
C	-4.1866489679	0.4792484809	1.0762722265
H	-5.0161320366	0.3498496063	0.3718982355
H	-4.4825000101	1.237889022	1.8064194654
H	-4.0456880807	-0.466100673	1.6078442889
C	2.1803954351	-1.2032837317	0.405052699
H	2.5372079349	-1.5190668156	1.3826318769
C	2.9197658752	-1.7049345702	-0.803697371
H	2.4876735261	-1.3087702534	-1.7248972074
H	2.9005148414	-2.7971901055	-0.8583774329
H	3.9628883703	-1.3857791056	-0.7493820148
C	2.476325936	2.2674085431	1.2718737929
H	2.1451071808	3.3083855945	1.1626054753
H	2.1186474914	1.9043966417	2.2390333133
H	3.5689503015	2.2691348053	1.2829994255
C	2.5520802098	1.7142332404	-1.2181810197
H	2.125334119	1.0662524942	-1.9873373883
H	2.3493280515	2.7546503492	-1.5032792318
H	3.6363445049	1.5769670535	-1.2085965618
H	3.6363445049	1.5769670535	-1.2085965618

TS 6-311++G(d,p) 0057

E(UwB97XD) = -1036.88792733 A.U.

First frequency = -1609.1801 cm⁻¹

S	0.3307276497	-1.2681015473	0.5031493054
O	-0.3670185216	-2.344668921	-0.1921055631
O	0.0863513469	-1.0906463463	1.9324275124
N	-0.0324611985	0.1390625017	-0.2718102744
C	0.6265938925	1.3346490825	0.2577312203
H	0.2187200488	2.193304631	-0.2843663478
H	0.3560427807	1.4622436669	1.3095906703
C	2.1466973416	1.282980219	0.1073697476
H	2.3376491782	0.0042205396	0.3123988464
C	-0.8159709853	0.1988581203	-1.5050361648

H	-1.0002293253	-0.8272179141	-1.8242518509
H	-0.2084627989	0.6787377632	-2.2803285147
C	-2.1474219125	0.935742346	-1.3721024951
H	-2.5889550991	0.9341989338	-2.3753721804
H	-1.9743117714	1.9902727556	-1.1220588425
C	-3.1461452895	0.3284651574	-0.3727084994
H	-3.0040526362	-0.7599667288	-0.374214878
C	-2.9236881702	0.8375816828	1.0540897377
H	-1.9231289827	0.6057957981	1.4204387713
H	-3.6445699136	0.3856534054	1.7419885067
H	-3.0607402955	1.924570206	1.0931208001
C	-4.5821607314	0.6198026821	-0.8139258873
H	-4.7557464471	1.7007277144	-0.867706046
H	-5.3038986654	0.2012630452	-0.1064535881
H	-4.7899406025	0.1969841132	-1.8011921551
C	2.0844544349	-1.371332229	0.3016660459
H	2.5413532172	-1.7743130547	1.2024674282
C	2.5610585036	-1.9087963749	-1.0190637535
H	3.6303607772	-1.7153500316	-1.1285314556
H	2.0436731923	-1.4335163311	-1.8557222548
H	2.4003323695	-2.9883395818	-1.091087714
C	2.9025637243	2.0250910127	1.1825214864
H	3.9807058909	1.8830836338	1.0745870242
H	2.7031336475	3.1028126886	1.1165729649
H	2.6056960585	1.6925956884	2.1806958276
C	2.6387442037	1.5250131702	-1.3016816121
H	2.5017966862	2.5802561851	-1.5708319672
H	3.7023611537	1.2916747646	-1.3960493198
H	2.0920667727	0.923116922	-2.0312644759
H	2.0920667727	0.923116922	-2.0312644759

TS 6-311++G(d,p) 0058

E(UwB97XD) = -1036.89117147 A.U.

First frequency = -1534.3514 cm^{-1}

S	0.6225454957	-1.3465183879	0.9009615037
O	-0.3625652084	-2.3874306189	0.6235337594
O	1.2992828879	-1.3956151877	2.1987048393

N	-0.1454928201	0.1224669145	0.6752891523
C	0.7283775069	1.2711088012	0.9827847722
H	0.1021670383	2.1663476097	0.9377819038
H	1.1274243006	1.197556437	2.0013104019
C	1.8569211551	1.3895900355	-0.0326366722
H	2.1003770228	0.1340401186	-0.2415981112
C	-1.5419788006	0.1927929057	1.1552206773
H	-1.7016787317	1.2251440708	1.4698729407
H	-1.6833493335	-0.4218789336	2.0501833174
C	-2.5627891539	-0.1985841678	0.0896484707
H	-3.5590723131	0.003756498	0.5044496081
H	-2.5020072465	-1.2765099895	-0.0786705548
C	-2.4184459429	0.524554369	-1.253053152
H	-1.4337206102	0.2668662585	-1.6590298509
C	-3.4770456513	0.0206487929	-2.2343469693
H	-4.4839452823	0.2636033105	-1.8765563082
H	-3.4179461599	-1.0647509721	-2.3569865135
H	-3.3521775784	0.4802024791	-3.2190444872
C	-2.4899189212	2.0453775008	-1.1142352248
H	-1.6692646609	2.4437598905	-0.5119138757
H	-3.4314654037	2.3479211478	-0.6419206162
H	-2.4363402202	2.5271051053	-2.0947543058
C	1.8667586415	-1.2431535	-0.3430212163
H	2.7726899015	-1.7270039624	0.0145924295
C	1.4250023436	-1.5339456413	-1.7495174172
H	1.214971339	-2.598379573	-1.8890761035
H	2.2165595795	-1.2492285405	-2.4459455072
H	0.5242216731	-0.9721185356	-2.0045636482
C	3.1266922681	1.9949141778	0.5153154454
H	3.4757638146	1.4564311077	1.400247702
H	3.9213056024	1.9855730012	-0.2346414305
H	2.9572182613	3.0401290037	0.8051577049
C	1.4133437484	1.9271479414	-1.374595026
H	1.2070282825	3.0023173499	-1.2963379641
H	2.1869470806	1.79022414	-2.1343321041
H	0.4989157995	1.4367266941	-1.7149354607
H	0.4989157995	1.4367266941	-1.7149354607

TS 6-311++G(d,p) 0060

E(UwB97XD) = -1036.88978886 A.U.

First frequency = -1547.0664 cm⁻¹

S	0.4121734521	-1.3215240528	0.2840063825
O	-0.0227272378	-1.6867945304	-1.0655720783
O	-0.0740014167	-2.1484082492	1.3866380684
N	0.0074735432	0.2479608285	0.6494574241
C	0.46292991	1.2384733945	-0.3385319186
H	0.1295052756	0.9766566962	-1.3486278901
H	-0.0067240116	2.1900031159	-0.0752686139
C	1.9788813208	1.3782195175	-0.3044753512
H	2.2900650413	0.1332711014	-0.1301416796
C	-1.2387872573	0.474205499	1.3978717164
H	-1.2401133373	1.5386983255	1.6427721119
H	-1.1541574717	-0.0646974183	2.3427964952
C	-2.5400129518	0.061421145	0.708281122
H	-3.3555729721	0.2539920877	1.4180004484
H	-2.5191065484	-1.0228460545	0.5557819678
C	-2.868603951	0.7472703195	-0.6224440992
H	-2.0287808884	0.5847765177	-1.3070542885
C	-4.1018296121	0.095193663	-1.2498932974
H	-4.9740923309	0.211200179	-0.5966809859
H	-3.9429443903	-0.9745326215	-1.4127570497
H	-4.3419599701	0.552972884	-2.213720291
C	-3.0862046876	2.2526401275	-0.4622289813
H	-3.3182268274	2.7162196867	-1.4251199524
H	-2.2091808465	2.7628283416	-0.0559604323
H	-3.9260023942	2.4469074133	0.2144365602
C	2.1749083773	-1.199389824	0.2737773622
H	2.5286154651	-1.1679515828	1.3025658114
C	2.9093440639	-2.0941267958	-0.6839583697
H	3.9693332248	-1.8319214551	-0.6764369482
H	2.5274122429	-1.979795808	-1.6994331043
H	2.8236638192	-3.1488148579	-0.4020264049
C	2.501784611	2.0705437583	0.932746499
H	2.262558978	3.1409216472	0.8957414355
H	2.048008597	1.6539973558	1.8356722601

H	3.5874693531	1.9734729056	1.0124432684
C	2.5936965381	1.8227594579	-1.6089034174
H	2.2813219634	2.8471126739	-1.8512131171
H	3.6848329796	1.8167375043	-1.5507046803
H	2.2857966575	1.1773336971	-2.4359564716
H	2.2857966575	1.1773336971	-2.4359564716

TS 6-311++G(d,p) 0061

E(UwB97XD) = -1036.88694487 A.U.

First frequency = -1598.7746 cm⁻¹

S	0.3035917018	-1.188942619	0.5549886319
O	0.0866706184	-1.9443001754	-0.6766911518
O	-0.4238895185	-1.6062282278	1.7501106662
N	-0.0569627945	0.3930867321	0.2801126694
C	0.6570176948	1.020674228	-0.8336052006
H	0.4566004821	0.4632836298	-1.7531342507
H	0.2309296833	2.0198415892	-0.9669005081
C	2.1617518131	1.1076854784	-0.5881421838
H	2.3365354025	-0.0352589987	0.0157528275
C	-0.8873749577	1.1938992302	1.1792036366
H	-0.2990589641	2.050191844	1.5266529867
H	-1.113089743	0.5783151771	2.0501227584
C	-2.1908559521	1.691705629	0.5570358213
H	-1.9777493417	2.3763511882	-0.2738280753
H	-2.6740715113	2.3005419784	1.3299154462
C	-3.1639270707	0.5989991653	0.0836082484
H	-3.0542542881	-0.2639505679	0.7531412245
C	-4.6080590028	1.0953439162	0.1832307079
H	-5.3115400301	0.3313007502	-0.1601766973
H	-4.7518953437	1.9857263173	-0.4396253567
H	-4.8692030591	1.3597102193	1.212092766
C	-2.8671381815	0.1359240786	-1.3453679867
H	-2.9708414639	0.9746734795	-2.0436363095
H	-3.5711852353	-0.643154667	-1.6527619365
H	-1.85918859	-0.2684680936	-1.4433432306
C	2.0507277621	-1.1342744186	0.8302048587
H	2.2329119054	-0.7416308621	1.8296506558

C	2.8556039394	-2.329726871	0.4052752253
H	3.9185677451	-2.1075972382	0.5214142738
H	2.662617724	-2.5810188922	-0.638603366
H	2.628788895	-3.2090069077	1.0174971809
C	2.5644774523	2.1264025717	0.4541975719
H	2.0113893298	1.985891246	1.3867157436
H	3.6316167592	2.0576872829	0.6799388488
H	2.3612769951	3.1423093096	0.0926859372
C	2.9970079744	1.1053968956	-1.8447185269
H	2.8232875628	2.0221612703	-2.4238335458
H	4.0630449441	1.0637248722	-1.608046081
H	2.7499283133	0.2557084305	-2.4867320905
H	2.7499283133	0.2557084305	-2.4867320905

TS 6-311++G(d,p) 0069

E(UwB97XD) = -1036.88692425 A.U.

First frequency = -1588.6300 cm⁻¹

S	0.2569207734	-1.2627772599	0.3948834273
O	0.1436607135	-1.875880211	-0.9260681108
O	-0.5187926348	-1.8419455048	1.4877420531
N	-0.1669673102	0.3238705915	0.2655545145
C	0.5916571624	1.0887052826	-0.7282497433
H	0.4483275624	0.6285652269	-1.7094918491
H	0.1465844776	2.0863563866	-0.7778608873
C	2.082341227	1.1869824214	-0.4062310784
H	2.2670416724	0.0013414814	0.1018252817
C	-0.9877539258	1.0062808908	1.2694005588
H	-0.3661754123	1.7061195616	1.8393918571
H	-1.3407088732	0.2476721698	1.9666887436
C	-2.1754702092	1.7716884873	0.6846184243
H	-1.8155208758	2.5905578204	0.0510575463
H	-2.6626844539	2.2529300204	1.541036527
C	-3.2335981609	0.9679532062	-0.091413149
H	-4.0815563839	1.6533822725	-0.2144155559
C	-2.7843890666	0.5648514638	-1.499767069
H	-2.3977412205	1.4273165166	-2.052055317
H	-3.6288224834	0.1580288868	-2.0644292347

H	-2.0023730079	-0.1964796827	-1.4711023559
C	-3.7363555877	-0.2437386676	0.695398615
H	-4.5847039888	-0.7077287474	0.1842598644
H	-4.0642685476	0.0425878087	1.6999332707
H	-2.9563726001	-1.0035005213	0.8002062004
C	1.9807561713	-1.1821431304	0.7858898925
H	2.0880416681	-0.8889984124	1.8294165523
C	2.8549601882	-2.3006323242	0.2934050126
H	2.7339435761	-2.4481232422	-0.780713835
H	2.6259885143	-3.2454645444	0.7976386745
H	3.8998241371	-2.0578062112	0.4983470444
C	2.4208955623	2.1232788173	0.7323529217
H	3.4842385864	2.0720712886	0.9796034346
H	2.1890424039	3.1594563573	0.4555322002
H	1.8529523109	1.8839757879	1.6349348559
C	2.9675765497	1.3108264166	-1.622518253
H	4.0240279416	1.2756484252	-1.3450960911
H	2.7703293819	0.5121314577	-2.3425013139
H	2.7916553733	2.2682892985	-2.1307502113
H	2.7916553733	2.2682892985	-2.1307502113

TS 6-311++G(d,p) 0074

E(UwB97XD) = -1036.89086926 A.U.

First frequency = -1528.5395 cm⁻¹

S	0.763207085	-1.6324056787	0.5124090966
O	0.0383948632	-2.7236615157	-0.1333395549
O	1.2256603477	-1.8556011879	1.8840852495
N	-0.2168772139	-0.2779159859	0.4112101514
C	0.3714911521	0.9142005665	1.0518702929
H	-0.3901408795	1.6974183833	1.014084305
H	0.586932827	0.714468338	2.1088067791
C	1.624153969	1.3872779252	0.3263877278
H	2.1182172351	0.2488586269	-0.0402139522
C	-1.6490024983	-0.5189281831	0.6867622046
H	-1.931597028	0.0497401971	1.5773578911
H	-1.7985298879	-1.5712034712	0.9318764667
C	-2.5240634184	-0.1681765635	-0.5117943989

H	-3.5506508534	-0.4852038899	-0.2860191022
H	-2.1846708747	-0.7753405338	-1.3578415911
C	-2.5409286458	1.3089437485	-0.920785619
H	-1.504339133	1.6346789166	-1.0621515162
C	-3.2616839276	1.4750943383	-2.2590613115
H	-3.2671233498	2.521612573	-2.576960964
H	-4.3031352995	1.1435541723	-2.1799255063
H	-2.7803606266	0.8844706671	-3.043898865
C	-3.1846820371	2.1960975233	0.1463429603
H	-2.6728340258	2.1302199063	1.1105557372
H	-4.2289662857	1.9056126383	0.3062006955
H	-3.1719349502	3.2454436487	-0.1613104758
C	2.1473991206	-1.0937823978	-0.4346336692
H	3.0561460294	-1.5073862041	-0.0036574508
C	1.9923652248	-1.1467390879	-1.9283408679
H	1.0443663167	-0.705869472	-2.2430598492
H	2.0296233523	-2.1766955255	-2.2949849797
H	2.8048810181	-0.5889076107	-2.3989168094
C	2.6463019383	2.0431890226	1.2235493528
H	2.2459176352	2.9767324501	1.6399081078
H	2.9168004412	1.3946494586	2.0608322838
H	3.5535298964	2.2923462701	0.667993742
C	1.3503682191	2.1122783398	-0.9720540627
H	0.6608241323	1.5485398999	-1.6040176547
H	0.8966207725	3.090652606	-0.7682669866
H	2.2731883792	2.281373622	-1.5324730176
H	2.2731883792	2.281373622	-1.5324730176

TS 6-311++G(d,p) 0077

E(UwB97XD) = -1036.88957489 A.U.

First frequency = -1523.1511 cm⁻¹

S	0.5164455401	-1.451707901	-0.4483988032
O	1.3205718268	-1.8281288943	-1.6133585282
O	-0.5629337904	-2.3615405424	-0.0740104964
N	-0.162975813	0.0624714438	-0.6417623069
C	0.8203486603	1.0819366933	-1.0575599339
H	1.3462808762	0.7712098954	-1.968197696

H	0.2551341145	1.9868722478	-1.2968812353
C	1.8078731544	1.3788476453	0.0622741334
H	1.9339788326	0.1935144229	0.5593069402
C	-1.4806941357	0.0884648856	-1.3127213531
H	-1.540416941	-0.6731566832	-2.0974695079
H	-1.5362377353	1.0517144597	-1.8218783112
C	-2.6550578641	-0.0629703418	-0.3477943021
H	-2.7055194825	-1.0999523892	-0.0083059478
H	-3.57112522	0.1302867412	-0.9214172405
C	-2.6189781585	0.8599326672	0.8741347595
H	-1.7157235831	0.6128246241	1.4440357888
C	-2.5495998058	2.3381327181	0.4900843294
H	-1.6336363213	2.5792899508	-0.0554157115
H	-2.5732374566	2.9724449195	1.3809128198
H	-3.4010328071	2.614590693	-0.1423027107
C	-3.8296465818	0.5903520611	1.7682535291
H	-4.7608315968	0.8316506268	1.2432090393
H	-3.7913706276	1.1977443367	2.6771710097
H	-3.8756634327	-0.4614234486	2.0654645677
C	1.6143691294	-1.1260688157	0.8931408823
H	1.032478747	-1.014657317	1.8060155075
C	2.861454455	-1.9608818696	0.9604487408
H	3.4067071297	-1.9286774929	0.01603291
H	2.6373970953	-3.0073437042	1.1927681261
H	3.5074621668	-1.5748500952	1.7515327642
C	1.2207918288	2.1905450078	1.1947320536
H	1.0428566128	3.2226509615	0.8670949775
H	0.2656711726	1.7730949045	1.5220888865
H	1.8991444729	2.2234689696	2.0509973249
C	3.173592361	1.8150353019	-0.4097024385
H	3.6014488245	1.095259734	-1.1126391543
H	3.1112230262	2.7843787795	-0.9213995389
H	3.860837268	1.9307776029	0.4318709698
H	3.860837268	1.9307776029	0.4318709698

TS 6-311++G(d,p) 0083

E(UwB97XD) = -1036.88868497 A.U.

First frequency = -1599.8584 cm⁻¹

S	0.5324229418	-1.4751636684	0.4315322453
O	0.5032530642	-2.2102126687	-0.829306079
O	-0.1403868831	-2.0562061065	1.5891570155
N	-0.1363174929	0.0111887516	0.173843824
C	0.5113601456	0.8021291756	-0.8780096244
H	0.4879763184	0.226805852	-1.8065279187
H	-0.1031786556	1.6924825672	-1.0396907023
C	1.9512157265	1.188144819	-0.5427604656
H	2.3232867426	0.0771570533	0.0327530475
C	-0.9545482204	0.6578209843	1.2096892405
H	-0.7330670335	1.7265951699	1.1726994921
H	-0.6451498091	0.3067958391	2.1960580669
C	-2.4462336495	0.4010339543	1.0169360694
H	-2.9853357625	0.8742063456	1.8481813531
H	-2.6154950884	-0.6772119351	1.1029132027
C	-3.0221804191	0.9023287249	-0.3118999026
H	-2.400405976	0.4947164782	-1.1188920037
C	-4.4435992194	0.3726222683	-0.5049908261
H	-5.1021808275	0.7346533026	0.2926440452
H	-4.4638542629	-0.7207358458	-0.4868706004
H	-4.8617909682	0.7038323709	-1.4598772355
C	-3.0048445715	2.4292971532	-0.4092825205
H	-3.4057609678	2.7621498004	-1.3707273263
H	-1.9975701571	2.8444677007	-0.3133216676
H	-3.6209831466	2.8704776274	0.3822349491
C	2.2277245456	-1.0985775351	0.7813909738
H	2.3001730349	-0.7360757603	1.8059479052
C	3.2645007093	-2.0888118734	0.3309196175
H	4.2591467395	-1.6712399717	0.5012645024
H	3.1561535782	-2.3132107939	-0.7311803034
H	3.1959155779	-3.0287752179	0.8886242122
C	2.0930933168	2.2262471373	0.5478347173
H	1.5730972008	1.9281413724	1.4619968859
H	3.1443378756	2.3907814003	0.7969408709
H	1.6709745789	3.1846995607	0.2195755791
C	2.8267721659	1.4053581744	-1.7525790123
H	2.4982960142	2.2920133627	-2.3110605449
H	3.8671787054	1.5684891946	-1.4607878507

H	2.78647139	0.55097209	-2.4334683496
H	2.78647139	0.55097209	-2.4334683496

TS 6-311++G(d,p) 0085

E(UwB97XD) = -1036.88734262 A.U.

First frequency = -1591.8900 cm⁻¹

S	0.8040466653	-1.7652087255	-0.0381417909
O	1.6406497895	-2.2361360388	-1.1352647142
O	-0.0937949815	-2.7133906276	0.6110258059
N	-0.133776385	-0.5190050016	-0.6381700695
C	0.6881009869	0.5266814801	-1.2803189369
H	1.2323388504	0.0408541025	-2.0904847438
H	0.0030742939	1.2392876003	-1.7442608757
C	1.6783650327	1.244352214	-0.3551441728
H	1.9160409176	0.2812429004	0.4922870765
C	-1.249309486	-0.1048056519	0.2375937386
H	-0.8806806204	0.3249366774	1.1768621771
H	-1.801387249	-1.0101776393	0.4912760615
C	-2.1887358042	0.8705056893	-0.4597844077
H	-2.4018066352	0.490159695	-1.4645927739
H	-1.7088649216	1.8491299567	-0.5807873719
C	-3.5084259889	1.0747255198	0.2949768945
H	-3.9926368219	0.0951424033	0.3970750305
C	-3.2887755314	1.6486945046	1.6967639426
H	-4.2460034786	1.8446216669	2.1876798004
H	-2.7402827774	2.5961046726	1.6414519395
H	-2.723559515	0.9683769715	2.3388517709
C	-4.4362339394	1.9795816979	-0.5163144245
H	-3.9941766803	2.9747068377	-0.6384215169
H	-5.4007831637	2.1013658821	-0.015786427
H	-4.620802031	1.5686311332	-1.5129631624
C	1.8520123157	-0.9553770026	1.1404792999
H	1.2815937111	-0.7519898886	2.0454161681
C	3.2386246804	-1.5076777856	1.3190827102
H	3.2224557597	-2.4962803689	1.7896494789
H	3.811687885	-0.8391902974	1.9649692605
H	3.7527789887	-1.5937027255	0.360697045

C	1.1154722667	2.3961720016	0.4496799994
H	0.2232755416	2.1201271179	1.0143150586
H	1.8578773309	2.7792429147	1.1543820886
H	0.8391265136	3.2194656058	-0.2217100085
C	3.0050370771	1.5449100991	-1.0151102293
H	2.8736616141	2.2736836578	-1.8256852959
H	3.7129767087	1.9715366144	-0.3000898174
H	3.4477772413	0.6440344789	-1.4482232598
H	3.4477772413	0.6440344789	-1.4482232598

TS 6-311++G(d,p) 0086

E(UwB97XD) = -1036.88969129 A.U.

First frequency = -1514.0989 cm⁻¹

S	0.6512642339	-1.6550655126	-0.1562881668
O	1.1954802195	-2.0580459593	-1.4553064124
O	-0.1658701506	-2.640795339	0.5482187672
N	-0.2720682694	-0.2636297049	-0.2813831369
C	0.4282610209	0.8439444985	-0.9610425756
H	0.76615145	0.5316114657	-1.9571644046
H	-0.3067263622	1.6407316896	-1.1005094391
C	1.5946844328	1.3620862663	-0.1330973619
H	2.019206629	0.2501431418	0.3620886737
C	-1.6723530943	-0.4897528839	-0.700874145
H	-1.8418181346	-1.5598657584	-0.8270044541
H	-1.8196524099	-0.034754885	-1.6848903473
C	-2.6682875501	0.0403704939	0.3254575736
H	-2.4608704043	-0.4605248729	1.2769698169
H	-3.6724343003	-0.2759511425	0.0138865692
C	-2.675125146	1.5582073873	0.5407642889
H	-1.6522408255	1.8756856191	0.7721218382
C	-3.1481645886	2.3146113587	-0.7019631639
H	-2.5265620902	2.1114174171	-1.5784879806
H	-3.1307522869	3.3944107844	-0.5297933151
H	-4.1761900465	2.0311636589	-0.9534967784
C	-3.5484762991	1.9122200461	1.7450712085
H	-3.5532778711	2.9910241316	1.9251415447
H	-3.1901240336	1.4182036282	2.652786875

H	-4.5840582765	1.5959946391	1.5766488043
C	1.9815277638	-1.0632657998	0.8392514667
H	1.6307167926	-0.9422696043	1.8620899618
C	3.3149348389	-1.7248320532	0.6353652694
H	3.6087174951	-1.7022303428	-0.41501369
H	3.3056145633	-2.7682654385	0.9675618458
H	4.0684457099	-1.1950846045	1.2215237052
C	1.1845697975	2.1604023403	1.0838040256
H	0.4482267817	1.6163204273	1.6805374202
H	2.0472268634	2.3824464059	1.7168851646
H	0.7360315683	3.1145293475	0.7794739054
C	2.7168669395	1.9556935554	-0.9496925385
H	2.3780691349	2.8656289785	-1.4622235649
H	3.5614879594	2.2310734408	-0.3136545162
H	3.0685981748	1.2562478395	-1.7126811708
H	3.0685981748	1.2562478395	-1.7126811708

TS 6-311++G(d,p) 0096

E(UwB97XD) = -1036.88719294 A.U.

First frequency = -1597.9939 cm^{-1}

S	0.6273481697	-1.4762691896	-0.0351715227
O	1.0889541654	-2.0830194347	-1.2794346324
O	-0.3796772318	-2.1805477236	0.7517992598
N	0.008041193	0.0127331583	-0.4004249444
C	0.9471556809	0.9125662097	-1.0815886978
H	1.2755980539	0.4277248974	-2.0032611939
H	0.3832563004	1.8044114694	-1.372504821
C	2.1643102986	1.2864608452	-0.2344571549
H	2.3600437468	0.1378315749	0.3528541532
C	-1.0904116013	0.5696935382	0.4037266056
H	-0.910187643	1.6429949969	0.4813553512
H	-1.059745552	0.1677476055	1.4206986241
C	-2.451613783	0.2956384534	-0.2251853798
H	-2.5508236184	-0.7857746912	-0.3599329247
H	-2.4778377484	0.7465068077	-1.2256791889
C	-3.6328266067	0.8136713293	0.6024001744
H	-3.5674175839	0.3592704196	1.6000887823

C	-3.6032100488	2.3351421285	0.7689899887
H	-4.484495264	2.6818819757	1.3159677201
H	-3.6014216211	2.8277326795	-0.2100879087
H	-2.7220381273	2.675937569	1.3189538617
C	-4.9520638634	0.3703464621	-0.0313140229
H	-5.8064552134	0.6946955247	0.5695971706
H	-4.9993026239	-0.717922268	-0.1292845427
H	-5.0623263121	0.8032539064	-1.031868964
C	2.0641187383	-1.0996127941	0.9308062699
H	1.7499994162	-0.8286492174	1.93790105
C	3.2414847773	-2.0256192349	0.8079468026
H	4.0888234242	-1.6050430567	1.3536295403
H	3.5279083187	-2.1572387886	-0.2363890616
H	3.0263723418	-3.0122181565	1.231755816
C	1.8854158422	2.2343427841	0.911068838
H	1.5559382846	3.2089119035	0.5289880929
H	1.1041178161	1.8549522879	1.5745281569
H	2.784862776	2.3962544866	1.5102722893
C	3.395691894	1.6114523766	-1.0448768405
H	3.6288249909	0.8135538999	-1.7549597726
H	3.2451519187	2.5351636071	-1.6193954626
H	4.2628802662	1.765119874	-0.3979423738
H	4.2628802662	1.765119874	-0.3979423738

TS 6-311++G(d,p) 0097

E(UwB97XD) = -1036.88802202 A.U.

First frequency = -1516.8516 cm^{-1}

S	0.6415356302	-1.2276045103	1.0319214233
O	-0.3611023747	-2.2783313504	0.8851314908
O	1.288000839	-1.1020750517	2.3400750259
N	-0.0903480813	0.2158690821	0.5759801964
C	0.8003534155	1.3787405868	0.7767702063
H	0.2142290997	2.2644156537	0.5146754356
H	1.0837243903	1.4697014567	1.8322842748
C	2.0413309835	1.3144689922	-0.1073242235
H	2.2214762875	0.0375201893	-0.1832874395
C	-1.4640806144	0.371828579	1.1130717396

H	-1.6055815277	1.4401763162	1.2936661253
H	-1.5449277185	-0.1111540257	2.0922686803
C	-2.5565367802	-0.1484276049	0.1776069857
H	-3.41125857	-0.4396019656	0.7982392365
H	-2.2025089812	-1.0634096121	-0.306117425
C	-3.0512938088	0.8435356628	-0.8810487663
H	-3.4410346402	1.7249496017	-0.3534740671
C	-1.9429304536	1.3130889649	-1.8225043435
H	-1.4653126463	0.4585333879	-2.3143035757
H	-1.1666406106	1.8679244293	-1.2926587493
H	-2.347546099	1.9686783485	-2.59932131
C	-4.2019966951	0.2239608625	-1.6754655583
H	-3.856550193	-0.6574668702	-2.2272544621
H	-4.6080878979	0.9348005137	-2.4007895155
H	-5.0166911161	-0.0912736481	-1.0169608532
C	1.9102345236	-1.3276012359	-0.1818778719
H	2.7762311935	-1.8281951403	0.2450111551
C	1.4763673153	-1.7219852391	-1.565035891
H	0.6028451401	-1.1474850891	-1.8803260429
H	1.2241889289	-2.7854000851	-1.6137822222
H	2.2878957305	-1.5324720446	-2.2708321025
C	3.2820462317	1.8893394542	0.534201205
H	3.1604494119	2.9673726195	0.7022273569
H	3.4824708248	1.4221577903	1.5018471452
H	4.1554851409	1.75198373	-0.1077510628
C	1.8077991673	1.7356130977	-1.5409405541
H	1.6188339306	2.8156771851	-1.5903326821
H	2.681343035	1.5204122208	-2.1614517976
H	0.9435330545	1.2254828461	-1.969803531
H	0.9435330545	1.2254828461	-1.969803531

TS 6-311++G(d,p) 0103

E(UwB97XD) = -1036.88678465 A.U.

First frequency = -1505.6764 cm⁻¹

S	0.4195485392	-1.4655009475	-0.4506389837
O	1.2005382265	-1.9204079305	-1.6032248873
O	-0.7287501044	-2.283686968	-0.0695537993

N	-0.1480820261	0.0915844974	-0.6750578879
C	0.9073388774	1.0370402573	-1.0919565609
H	1.4050485948	0.6892861586	-2.0053886395
H	0.4043525982	1.9793234651	-1.3255727582
C	1.9185954082	1.2668197488	0.0225636475
H	1.9401954284	0.08947869	0.548097902
C	-1.4313746425	0.180109643	-1.4075536336
H	-1.518681924	-0.6235293456	-2.1466111072
H	-1.3854604849	1.1121119247	-1.9744851434
C	-2.661521314	0.2062883846	-0.5054992509
H	-2.8186701908	-0.782444116	-0.0663883236
H	-3.5160344049	0.3950298424	-1.1652771565
C	-2.614722502	1.2711827904	0.6068682294
H	-1.9202567584	2.0623382593	0.2934756931
C	-3.9892452754	1.9097170867	0.8141797388
H	-4.7282773699	1.1486117301	1.088544172
H	-4.3396884876	2.4041489182	-0.0965467398
H	-3.9626589856	2.6535360976	1.6161813717
C	-2.1001794387	0.6850444212	1.9234000285
H	-1.9874181293	1.4623643846	2.6855856112
H	-1.1355009338	0.1946413253	1.7847853702
H	-2.8038225715	-0.0626308538	2.3057642665
C	1.5293411715	-1.2011879741	0.8947174521
H	0.9539938282	-1.0454368175	1.8052806484
C	2.7180641171	-2.1161803422	0.9753089552
H	3.3827119743	-1.7686924206	1.7687651743
H	3.2702828555	-2.1255255457	0.0344971756
H	2.4236702874	-3.1441170813	1.2116310682
C	1.4111471692	2.1623869817	1.1302473254
H	1.3558894355	3.2002600944	0.7780436553
H	0.4113079664	1.8623219833	1.4512427967
H	2.0775847239	2.1386828486	1.9962225077
C	3.3193775039	1.5606186554	-0.4576693986
H	3.3463329428	2.5145554928	-1.0003692275
H	4.0134901392	1.6398373687	0.3825288123
H	3.6798779611	0.7824007862	-1.1356378495
H	3.6798779611	0.7824007862	-1.1356378495

TS 6-311++G(d,p) 0127

E(UwB97XD) = -1036.88081670 A.U.

First frequency = -1541.5430 cm⁻¹

S	0.2920029464	-1.2762083401	0.3984368658
O	0.1349810623	-1.650824357	-1.0064406115
O	-0.4115393269	-2.1229478668	1.3627815836
N	-0.2105229209	0.2821182554	0.6448704353
C	0.6683483381	1.4490254278	0.4563687258
H	0.0787916469	2.227466424	-0.0418138529
H	0.9353550803	1.8276982977	1.4516921638
C	1.9358838631	1.2096434745	-0.3462995386
H	2.2427705333	0.0314039619	0.0952556934
C	-1.3871354355	0.5342993474	1.482434591
H	-1.0507970841	0.9787959778	2.4289039633
H	-1.8388726093	-0.4250055955	1.7270504287
C	-2.4313174227	1.4557388326	0.8498392976
H	-2.0146000299	2.459148926	0.708717974
H	-3.2161692599	1.5650780505	1.6075654642
C	-3.0836836272	0.9904837555	-0.4640717636
H	-3.9589321436	1.6379333001	-0.5999500273
C	-2.1876323462	1.1893741127	-1.6904225832
H	-1.8205339761	2.2190888331	-1.7482424123
H	-2.7473304262	0.9838373486	-2.6079986966
H	-1.3268702884	0.5188634833	-1.6650964903
C	-3.5904730848	-0.4507669734	-0.3825232733
H	-2.7619988647	-1.1639039608	-0.3346212408
H	-4.1839522049	-0.6994420271	-1.2667464704
H	-4.2195716903	-0.6037471168	0.5001025755
C	2.0220429758	-1.185012565	0.72794676
H	2.1756384596	-0.9693547092	1.7843413271
C	2.8762484477	-2.2530919717	0.1051324088
H	3.9272020877	-2.0272740141	0.2960158254
H	2.7188014116	-2.3010816463	-0.9733014923
H	2.6630609746	-3.2400538446	0.5290195209
C	3.0701929727	2.1191501743	0.0692941773
H	3.9781559815	1.890265062	-0.4933645708
H	2.8120515857	3.167352256	-0.1300528739

H	3.2893735144	2.0275754867	1.1363960758
C	1.743409562	1.0920585476	-1.8426248596
H	2.6756309861	0.7976830732	-2.3312380046
H	0.9744925179	0.362819788	-2.0991773474
H	1.4429290219	2.0649678268	-2.2525321221
H	1.4429290219	2.0649678268	-2.2525321221

6.2 1,6 HAT

6.2.1 Starting TS

TS input

$E(\text{UwB97XD}) = -1036.74769056 \text{ A.U.}$

First frequency = $-1414.9124 \text{ cm}^{-1}$

S	0.0016658848	1.5396656511	-0.0236213291
O	-1.1762254625	2.2325237948	0.5104606667
O	0.8622703694	2.2727684352	-0.9614147386
N	-0.5436547823	0.1289594044	-0.7191893867
C	-1.9967481211	-0.0036884329	-0.9342292481
H	-2.4400824438	0.980948911	-1.1036770345
H	-2.1303699571	-0.5764652055	-1.8578997905
C	-2.7337691688	-0.7039701321	0.2110410612
H	-2.5340463256	-0.132623717	1.1264064033
C	0.3920725854	-0.5825429967	-1.6109725658
H	0.9432782052	0.139434146	-2.2230068167
H	-0.2238521516	-1.1694159317	-2.2942130801
C	1.3544841871	-1.5330013643	-0.8911103749
H	1.8359396885	-2.1558971185	-1.6603065302
H	0.7691556254	-2.2119406714	-0.2622035979
C	2.4465617673	-0.8771143192	-0.0571651503
H	1.8295611589	0.0281731316	0.6123971818
C	3.0377844971	-1.7927711672	0.9957914613
H	2.2586643176	-2.2291842319	1.6291511012
H	3.744320214	-1.2552808023	1.6361827619
H	3.5823538428	-2.6196506549	0.5190591909
C	3.4831476283	-0.1088838175	-0.8544191008
H	4.175177446	0.4168970092	-0.1892803994

H	3.0244522442	0.6319043819	-1.5149682204
H	4.0716189082	-0.8005020595	-1.4727141946
C	1.036930057	0.9754975862	1.2853634835
H	1.7286157746	1.7736412202	1.5554604645
C	0.3541450625	0.2480681543	2.4108496597
H	-0.2275517135	-0.5984020656	2.0349493563
H	-0.3190298829	0.9070955518	2.9698786607
H	1.1087741081	-0.1347811484	3.1028754364
C	-2.2464602343	-2.1383229975	0.4099909693
H	-2.4189956248	-2.7361991242	-0.4937526717
H	-1.1764882751	-2.1688462198	0.6339599354
H	-2.7759082816	-2.6190506632	1.2386030193
C	-4.2394889447	-0.665319044	-0.0600849251
H	-4.4828263902	-1.2033729562	-0.984577016
H	-4.7934605143	-1.1385483801	0.7563188851
H	-4.6008322979	0.3632398437	-0.162242527
H	-4.6008322979	0.3632398437	-0.162242527

6.2.2 Lowest TS

6311Gdp TS-relax-1-6-0001

E(UwB97XD) = -1036.89757430 A.U.

First frequency = -1485.3597 cm⁻¹

S	0.0397371108	1.3307895706	-0.6750509568
O	-1.0161999307	2.2649983932	-0.2983182245
O	0.5647006259	1.3740809975	-2.0356131597
N	-0.5548053924	-0.190069088	-0.4329537733
C	-1.5335519925	-0.4425575733	0.628129556
H	-1.085954916	-1.0958083965	1.3869780872
H	-1.7698590011	0.5060868214	1.1134501952
C	-2.8336718375	-1.0674675945	0.1095817442
H	-2.5897126764	-2.0197143968	-0.3767203055
C	0.2105672583	-1.3358192699	-0.9382987217
H	0.5722842562	-1.0896898171	-1.9367356258
H	-0.5047504364	-2.1507314316	-1.0630770144
C	1.3559725365	-1.7990351829	-0.0313133804
H	1.6755913623	-2.7912118659	-0.3798255631

H	0.973055862	-1.9434196495	0.9846982422
C	2.5727426715	-0.8872086743	0.0075309574
H	2.0843331048	0.2948576871	0.1860426193
C	3.4599847632	-1.1136840286	1.2128569631
H	4.2636040847	-0.3735863323	1.2573380365
H	3.9250660085	-2.1068110239	1.1622384386
H	2.8903109457	-1.0616241439	2.1449248248
C	3.3305757258	-0.7774947189	-1.2994616931
H	3.7769542655	-1.7456099696	-1.5605566409
H	4.1404052719	-0.0476820005	-1.2184444574
H	2.6843061598	-0.4682878465	-2.1238170068
C	1.419065488	1.5083425358	0.4130769653
H	2.0842046363	2.2775401334	0.0249401092
C	1.1071610525	1.5457458546	1.8842436601
H	0.57746461	0.6446794349	2.2045130183
H	0.4955568251	2.4138049778	2.1479380655
H	2.0402316589	1.6025830656	2.4482825196
C	-3.5202801277	-0.1656537741	-0.9121032658
H	-3.7963028152	0.790908241	-0.4562869693
H	-2.8626957839	0.0450499247	-1.7585465426
H	-4.4301976195	-0.6372602358	-1.2931682087
C	-3.7481058609	-1.368614452	1.2970571143
H	-4.6711867726	-1.8492164382	0.963391477
H	-3.2637168146	-2.0330629018	2.0187522926
H	-4.0216904844	-0.4447638757	1.8184261465
H	-4.0216904844	-0.4447638757	1.8184261465

6.2.3 Additional TS

TS 6-31++G(d,p) 0001

E(UwB97XD) = -1036.75082395 A.U.

First frequency = -1470.8980 cm⁻¹

S	0.0407250566	1.335248725	-0.6771546977
O	-1.0184178984	2.2744912247	-0.2972825683
O	0.5702526206	1.3811551445	-2.0427077682
N	-0.5596128931	-0.1875859549	-0.4406349813
C	-1.5357804549	-0.4382392549	0.6248980499

H	-1.0846036192	-1.0893750995	1.3856736451
H	-1.7721608923	0.5138132233	1.106444477
C	-2.8376715061	-1.0683359627	0.1116130291
H	-2.5939292578	-2.0238076577	-0.3718579125
C	0.2095266985	-1.3330713671	-0.944877152
H	0.5727950002	-1.0847516335	-1.9437169745
H	-0.50618204	-2.149418626	-1.0698624991
C	1.3559143808	-1.7986924322	-0.0369821343
H	1.6759971167	-2.7906700894	-0.3895712192
H	0.9715224463	-1.9470897406	0.9794324614
C	2.5751725555	-0.8869262454	0.0070354271
H	2.0865841899	0.2954172944	0.1857932608
C	3.4597831569	-1.1164921605	1.216210046
H	4.2632978658	-0.3747748991	1.265027686
H	3.9260792304	-2.1101696036	1.1637748463
H	2.8867712671	-1.0673237309	2.1478045187
C	3.3400847459	-0.778290609	-1.2981757202
H	3.7910933445	-1.7469446996	-1.5539146237
H	4.1479969582	-0.044831085	-1.2149551386
H	2.6963690765	-0.4736895296	-2.1278624806
C	1.4210949616	1.5085167744	0.413262097
H	2.0888971539	2.2806079949	0.0306664135
C	1.1089971368	1.5438886095	1.8863829073
H	0.5809572671	0.6406232519	2.2072018787
H	0.495073183	2.4112910685	2.1515129185
H	2.0439431216	1.6022465564	2.4493155486
C	-3.5297525125	-0.1717108499	-0.9133028538
H	-3.8077250649	0.7872101087	-0.460702019
H	-2.8733592135	0.0367826682	-1.7629194547
H	-4.4402250153	-0.6482214618	-1.2903315738
C	-3.7494656122	-1.3668509994	1.3041210538
H	-4.6729356503	-1.8518325806	0.9738399642
H	-3.2612639996	-2.0281796213	2.0279939024
H	-4.0246490818	-0.4406337947	1.8229071632
H	-4.0246490818	-0.4406337947	1.8229071632

TS 6-31++G(d,p) 0003

E(UwB97XD) = -1036.75058266 A.U.

First frequency = -1498.8748 cm⁻¹

S	-0.115294067	1.438406552	0.6129489832
O	0.4349690397	1.4825642501	1.969448429
O	-1.1388740504	2.4213769012	0.243640011
N	-0.7922428218	-0.0676073417	0.4096959547
C	-1.5103074727	-0.2886251906	-0.85472828
H	-1.979260629	0.6590057441	-1.1312424034
H	-0.813368822	-0.5636801626	-1.6601483192
C	-2.6020965526	-1.3578875008	-0.7386113127
H	-2.1289881481	-2.3225283759	-0.5126745258
C	-0.0672362636	-1.2142485647	0.9826036698
H	-0.820223474	-1.9681254915	1.2277700893
H	0.3610149444	-0.8880700704	1.9312610919
C	1.0025576119	-1.8395119068	0.0780658745
H	0.5475983073	-2.1390447228	-0.8729388003
H	1.3303372627	-2.7712055529	0.5621329917
C	2.2263216785	-0.9714509884	-0.1861217331
H	1.754763599	0.2163118231	-0.4022417251
C	3.1334803712	-0.7801167485	1.014607539
H	3.9402448447	-0.0762395761	0.7877001647
H	3.5934541739	-1.7367870705	1.2974806812
H	2.5878944482	-0.3973508437	1.8821695599
C	2.9609756646	-1.3201047816	-1.4646019884
H	2.2864953356	-1.3071725555	-2.3271006509
H	3.3940601291	-2.3274907692	-1.3938596166
H	3.7799544233	-0.6192790433	-1.6550581732
C	1.2288820846	1.5085317415	-0.533944287
H	0.8313218947	1.5252638599	-1.5498901193
C	2.3272146348	2.4930786949	-0.2297964952
H	1.9862018922	3.5293051875	-0.3354857845
H	3.1512252775	2.337126898	-0.9314213454
H	2.7048568225	2.3561386517	0.7862081911
C	-3.3013723755	-1.4958422624	-2.0932921675
H	-4.0559412238	-2.2872082463	-2.0581226766
H	-3.8060162064	-0.5618261927	-2.3670376066
H	-2.5901524438	-1.7431299677	-2.8884955714
C	-3.5964981947	-1.0265971158	0.373524455

H	-4.3680112166	-1.7996205345	0.4432661205
H	-3.1004276457	-0.9460150449	1.3448538163
H	-4.0909868781	-0.0690731119	0.1715161431
H	-4.0909868781	-0.0690731119	0.1715161431

TS 6-31++G(d,p) 0023

E(UwB97XD) = -1036.74946496 A.U.

First frequency = -1489.8414 cm⁻¹

S	-0.1385346976	1.3889934805	0.6843466621
O	0.708963786	1.6337946985	1.8571537799
O	-1.2696856073	2.293713402	0.4491035275
N	-0.7398791955	-0.1464477755	0.7678521289
C	-2.1583022407	-0.430184346	0.5404907167
H	-2.58537857	-0.8169435758	1.4754954423
H	-2.6585378151	0.5154882629	0.3214915504
C	-2.4252273737	-1.4237781888	-0.5970836894
H	-1.9318062132	-2.3738708651	-0.3504396714
C	0.1175707245	-1.2092297092	1.3068687596
H	-0.5525083949	-1.9448473743	1.7609820194
H	0.7272466169	-0.7982709043	2.1160496327
C	0.9999534352	-1.902537127	0.2610512252
H	0.3633114996	-2.2920943326	-0.5399486797
H	1.4638772122	-2.7756582788	0.7445493343
C	2.1020300623	-1.0373442893	-0.3361986664
H	1.5326093342	0.1014481926	-0.5732909835
C	3.222362972	-0.6870534032	0.6246357963
H	2.8455830216	-0.2213014182	1.5400118622
H	3.9318426255	0.0065101096	0.1625800817
H	3.7757144219	-1.5930329292	0.9073738151
C	2.5802133053	-1.5076260534	-1.6948184551
H	3.3106572003	-0.8123246891	-2.1203929086
H	1.7468013017	-1.606955213	-2.3981830857
H	3.0647516777	-2.4902858496	-1.6108430789
C	0.9199200661	1.3517398981	-0.7285501811
H	0.3078501982	1.2320091796	-1.6229721267
C	2.0037880899	2.3946543307	-0.790799291
H	1.5935077966	3.4021477886	-0.9255429912

H	2.6552718898	2.1812731671	-1.6427902892
H	2.6073470145	2.3872108528	0.1197573527
C	-1.8756555672	-0.9216630567	-1.9316230058
H	-2.0978042338	-1.6310612345	-2.7348027043
H	-2.3246769631	0.0432053698	-2.1967730279
H	-0.7904904229	-0.7897926633	-1.8933433511
C	-3.9306864157	-1.6879483394	-0.6802953003
H	-4.472187997	-0.7687254076	-0.9337912756
H	-4.1522051172	-2.431294051	-1.4519044657
H	-4.3248936137	-2.0609374408	0.2708533212
H	-4.3248936137	-2.0609374408	0.2708533212

TS 6-31++G(d,p) 0025

E(UwB97XD) = -1036.74905115 A.U.

First frequency = -1450.6989 cm^{-1}

S	0.0486565539	1.5119244494	-0.5866256361
O	-0.998011912	2.4420418002	-0.1482495638
O	0.7047090686	1.7751426717	-1.874947652
N	-0.6174138217	-0.0150038815	-0.5732222557
C	-2.0790850909	-0.1581876543	-0.5749918824
H	-2.5101612103	0.7722631778	-0.2004972809
H	-2.4341504453	-0.2996745952	-1.6057809552
C	-2.5586431568	-1.3216785581	0.3013001503
H	-2.0990505815	-2.249824747	-0.0655008
C	0.1494261408	-1.0715954779	-1.2572548106
H	0.7295872797	-0.636021444	-2.0767839718
H	-0.5782247978	-1.7438713624	-1.7184081454
C	1.0505292874	-1.864510028	-0.3072560923
H	1.4009378983	-2.7617271672	-0.8387972058
H	0.444792656	-2.2125540487	0.5361732697
C	2.263060803	-1.0963306498	0.2023793802
H	1.830419132	0.099943795	0.4090456344
C	2.7676486941	-1.5621592555	1.5525083418
H	3.1557435507	-2.5877048133	1.4805589628
H	1.9664793983	-1.5614809167	2.2987325162
H	3.580124345	-0.9243947104	1.9150656288
C	3.3575314789	-0.8936360785	-0.8285796095

H	4.1342045728	-0.22250149	-0.4487770148
H	2.9697591579	-0.4669410347	-1.7585811565
H	3.8318292287	-1.8541796582	-1.0707181316
C	1.3257088745	1.3942908561	0.6248961486
H	2.1432092825	2.0565463157	0.3402958779
C	0.8844491561	1.4385245196	2.0627497819
H	1.7384428451	1.2152541629	2.7079459613
H	0.1028168483	0.7010020006	2.2605167699
H	0.4998213495	2.4269370366	2.3346513687
C	-4.0757126646	-1.4609353742	0.1514306383
H	-4.3626865627	-1.6172682485	-0.8936917071
H	-4.4458113216	-2.3099550965	0.7338808737
H	-4.5852737686	-0.5591317108	0.5112753689
C	-2.1606976069	-1.1345820517	1.7646436944
H	-2.5374519949	-1.9599502848	2.376837986
H	-1.0739625136	-1.0986577696	1.8783577623
H	-2.5739417411	-0.1997450693	2.162268328
H	-2.5739417411	-0.1997450693	2.162268328

TS 6-31++G(d,p) 0035

E(UwB97XD) = -1036.74987872 A.U.

First frequency = -1472.4461 cm⁻¹

S	0.0993341968	1.15365222	-1.0089247259
O	-0.9129536379	2.1975995961	-0.8225821308
O	0.60785454	0.8893535426	-2.3577951522
N	-0.5649587237	-0.2491379507	-0.4479880165
C	-1.5872110129	-0.1960004564	0.6067588193
H	-1.404196809	-1.0428710585	1.2802185305
H	-1.4627829089	0.7126960942	1.2015283706
C	-3.025102047	-0.2500437633	0.0774898715
H	-3.1671191141	0.6381140917	-0.5499745959
C	0.1406999252	-1.5160904978	-0.6824286578
H	0.5136946214	-1.5122921699	-1.7086770086
H	-0.6172639339	-2.3008322857	-0.6295409315
C	1.2632508915	-1.8240389896	0.3165576829
H	1.5275087559	-2.886486342	0.2051865266
H	0.871653408	-1.7106408854	1.3351013217

C	2.5306115018	-0.9939472557	0.1597469944
H	2.1077405817	0.222309462	0.0534082685
C	3.4059123268	-0.9835437374	1.3970460834
H	4.2471942748	-0.2929782407	1.2807611028
H	3.819580242	-1.9851619136	1.5790990727
H	2.8393794662	-0.6914703194	2.287180714
C	3.2957390875	-1.2322777254	-1.1280129753
H	2.6671410413	-1.0948596654	-2.0121124519
H	3.6924339964	-2.2566110039	-1.1480740502
H	4.1425110866	-0.543900226	-1.2096090943
C	1.5097655379	1.4886710984	0.0042051233
H	2.205964982	2.1178826747	-0.550721218
C	1.2418595383	1.8684998578	1.4371301758
H	0.7231715123	1.0684337051	1.9744665503
H	0.6390174386	2.779826643	1.5120111513
H	2.1940075058	2.0459682478	1.9432802801
C	-3.9968731851	-0.1755499975	1.2571802455
H	-3.879700378	-1.0459440333	1.9146850577
H	-3.8314659724	0.7260434958	1.8566472282
H	-5.0329564279	-0.1605677293	0.9056641762
C	-3.2830197182	-1.4913889685	-0.7762430065
H	-2.6220938485	-1.5199588609	-1.6477553045
H	-3.1258073017	-2.4073057265	-0.1923450826
H	-4.3155249442	-1.5000195565	-1.1393419573
H	-4.3155249442	-1.5000195565	-1.1393419573

TS 6-31++G(d,p) 0036

E(UwB97XD) = -1036.74769056 A.U.

First frequency = -1414.9771 cm^{-1}

S	-0.0353824085	1.4178242528	-0.331098641
O	-1.125807	2.2543159066	0.1826919515
O	0.6662416074	1.871162338	-1.5392959088
N	-0.6655769802	-0.1052972316	-0.5640174995
C	-2.1331019408	-0.2460387046	-0.5204908562
H	-2.6066420509	0.678041097	-0.8619648848
H	-2.39914266	-1.025779413	-1.2418234746
C	-2.6815971181	-0.619694192	0.8596446747

H	-2.3513849539	0.1546904543	1.5635659281
C	0.1315601421	-1.0416552144	-1.3794374731
H	0.5768219857	-0.5096180705	-2.2269877379
H	-0.5747587922	-1.7618133161	-1.795476279
C	1.2010228535	-1.8109913706	-0.5970227451
H	1.5667839338	-2.6183202645	-1.2496316398
H	0.7242016065	-2.2962108815	0.2610526643
C	2.4000874214	-1.0000563642	-0.1248616384
H	1.8825603766	0.0599672388	0.3820409822
C	3.1525745522	-1.6425986817	1.0230110082
H	3.6268605889	-2.5769218692	0.6918772039
H	2.482428149	-1.8861747764	1.8537955294
H	3.9425150984	-0.9834246703	1.3967415666
C	3.2967536443	-0.4830458818	-1.2334690935
H	3.7918567121	-1.3226930688	-1.7402113938
H	4.0761041349	0.1714553166	-0.8309750262
H	2.7362911927	0.0835009833	-1.9820683162
C	1.1914004457	1.166686072	0.908014813
H	1.9081342771	1.9869374702	0.8645369341
C	0.6938752257	0.7604421867	2.2679681689
H	0.1064415177	1.5561731679	2.7388504947
H	1.5482038605	0.539949735	2.9132911818
H	0.0704533775	-0.1360325156	2.2058332652
C	-2.155785685	-1.9732627463	1.3348170682
H	-2.4571261335	-2.7712313926	0.644588538
H	-1.0640065736	-1.9776216422	1.3974837659
H	-2.5491281122	-2.2185839017	2.3263372432
C	-4.2113064771	-0.6068338525	0.8146687577
H	-4.5863306317	-1.3500432516	0.1002470407
H	-4.630816425	-0.8471866952	1.7962937859
H	-4.5940031716	0.3741499832	0.5144157127
H	-4.5940031716	0.3741499832	0.5144157127

TS 6-31++G(d,p) 0038

E(U_wB97XD) = -1036.74736516 A.U.

First frequency = -1465.3598 cm⁻¹

S	-0.1023863868	1.2588197009	-0.4641024432
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O	-1.1166215436	2.1420969718	0.1212064547
O	0.069138709	1.2635601002	-1.9212641811
N	-0.4255632185	-0.2824478305	0.0494511342
C	-1.5588429951	-0.5511460567	0.9391118974
H	-1.2005862261	-1.2384029999	1.717141839
H	-1.8336901185	0.3855998347	1.4284255538
C	-2.7936827509	-1.154624305	0.2543648927
H	-2.5088805322	-2.1254762875	-0.1730399968
C	0.1020717028	-1.4354821067	-0.6987175492
H	-0.5169425024	-1.6371069159	-1.5815530443
H	-0.0196542545	-2.2849772358	-0.019102644
C	1.5692496251	-1.349370268	-1.1334363391
H	1.6544726557	-0.7263483576	-2.0286296334
H	1.8649538087	-2.3651175939	-1.4338024928
C	2.5395337627	-0.8349528014	-0.0830833656
H	2.1246733861	0.3728822147	0.083865672
C	2.441495652	-1.4967661393	1.276159678
H	2.7051870255	-2.561085038	1.2003014194
H	1.4307007469	-1.4304510195	1.6896167093
H	3.1302016922	-1.0326642489	1.9887242759
C	3.9555524739	-0.681945906	-0.5996931223
H	3.9793014646	-0.1073355858	-1.5311426138
H	4.3978471007	-1.66712146	-0.8021666633
H	4.5911720723	-0.1766805686	0.1343368801
C	1.4723799223	1.602890369	0.2621226154
H	2.0101049829	2.3277118724	-0.3489360272
C	1.4601206934	1.832031035	1.7500192039
H	2.4889744723	1.8604723229	2.1191572114
H	0.9364370175	1.0229815629	2.2684267139
H	0.9755787986	2.7786898219	2.0104883467
C	-3.3170372323	-0.2670059246	-0.8740748252
H	-4.1925635432	-0.7234442933	-1.3464974363
H	-3.6070716595	0.7170508739	-0.489617816
H	-2.5599191831	-0.1112929311	-1.6493552531
C	-3.8709920348	-1.4082326385	1.3116100111
H	-4.7457533318	-1.8918194516	0.8664340969
H	-3.5009700445	-2.0545580287	2.1148505655
H	-4.2018813361	-0.4645225292	1.7616000961

H -4.2018813361 -0.4645225292 1.7616000961

TS 6-31++G(d,p) 0039

E(UwB97XD) = -1036.74591605 A.U.

First frequency = -1491.1041 cm^{-1}

S	-0.0491099305	1.4410536004	0.7243009452
O	0.6366450031	1.4229232135	2.0181665985
O	-1.073582208	2.465106045	0.4951082804
N	-0.7897425537	-0.0398365298	0.5456535834
C	-1.664935779	-0.1894891935	-0.6294668275
H	-2.0604103257	0.8045706943	-0.8420555248
H	-1.0914151788	-0.508954537	-1.5128652061
C	-2.8444257747	-1.1564092257	-0.3938600413
H	-3.045064582	-1.1688886867	0.6845827978
C	-0.0412687676	-1.2207215656	1.0079756628
H	-0.7879842374	-1.9683014013	1.2860068277
H	0.4684513007	-0.9431408611	1.9314923741
C	0.9426542176	-1.8225824125	-0.0040308008
H	0.4150680026	-2.053045389	-0.9362998342
H	1.2746008863	-2.7896604073	0.4021619084
C	2.1705345395	-0.9754489012	-0.3118664655
H	1.7063676499	0.2213676257	-0.4750837231
C	3.1488592989	-0.8336069478	0.8385633792
H	3.9647518154	-0.1530758726	0.5758442659
H	3.5916020242	-1.8094276425	1.0807874945
H	2.6664461933	-0.4464663184	1.740601321
C	2.8237293372	-1.3082324419	-1.6380719489
H	2.1022400875	-1.2611083938	-2.4602832053
H	3.2385081274	-2.3255126101	-1.6151746147
H	3.6454818286	-0.6196228864	-1.8586103386
C	1.1741602011	1.5157878026	-0.5495688896
H	0.6773585654	1.540161664	-1.520839111
C	2.3023231084	2.4930288303	-0.3486808311
H	1.9571695517	3.53168093	-0.4057143705
H	3.0485796912	2.3430303752	-1.1336497889
H	2.782510366	2.341384429	0.6209561099
C	-2.5522025007	-2.58556045	-0.8666438674

H	-1.6855207402	-3.0298001982	-0.3702593239
H	-3.4118244194	-3.2349165187	-0.673937253
H	-2.3601032594	-2.596869929	-1.9461935337
C	-4.0917261611	-0.6212095679	-1.1061695842
H	-3.9100968685	-0.5240032617	-2.1834787785
H	-4.9385805535	-1.301087628	-0.9710762267
H	-4.3786407943	0.3620022741	-0.7204676269
H	-4.3786407943	0.3620022741	-0.7204676269

TS 6-31++G(d,p) 0047

E(UwB97XD) = -1036.74574453 A.U.

First frequency = -1512.4594 cm^{-1}

S	-0.2096139196	1.4308281452	0.6902567621
O	0.7418893461	1.8665021999	1.7159000637
O	-1.4015009252	2.2490266351	0.4458387845
N	-0.744946934	-0.0726602845	1.1249953736
C	-1.9971294553	-0.5966739016	0.5632320506
H	-2.2476942925	-1.4495006526	1.2016136437
H	-2.7761336407	0.1532522554	0.7219681777
C	-1.987023329	-1.0386217904	-0.9245399064
H	-0.9433429635	-1.1093276682	-1.2508138588
C	0.2298541356	-1.0276559897	1.6702326194
H	-0.3278280687	-1.6782999868	2.350567527
H	0.9365491046	-0.465007193	2.2831624938
C	0.9713518168	-1.8885846167	0.639034455
H	0.2433258769	-2.4464009345	0.0407040622
H	1.5442681139	-2.6422476072	1.1997485456
C	1.9293575204	-1.1302450793	-0.2713176942
H	1.3187024701	-0.023510973	-0.5720426286
C	3.1941427118	-0.6494505108	0.4152922783
H	3.7960284539	-0.0312705234	-0.2579209848
H	3.8082892835	-1.507347561	0.7209616272
H	2.9738192885	-0.057285855	1.3087353335
C	2.1705683993	-1.8005651303	-1.6083667418
H	2.6842178838	-2.7615462266	-1.4669094968
H	2.7980501136	-1.1798982298	-2.2557463585
H	1.2289550068	-2.0017017192	-2.1302827422

C	0.6999504857	1.2091377994	-0.8125562539
H	0.0053062935	0.9911569377	-1.6240858381
C	1.7711010617	2.2240417172	-1.1130135567
H	2.3323070929	1.8991400827	-1.9935549378
H	2.4640999964	2.3232951442	-0.2746635032
H	1.3470316871	3.211241578	-1.3297891533
C	-2.7006254345	-0.0203483798	-1.8203327281
H	-2.2912542973	0.9868624736	-1.7004846029
H	-2.6207526182	-0.3047847948	-2.8743043655
H	-3.7656246998	0.0280652772	-1.5640779809
C	-2.6183571926	-2.4248752517	-1.0780992606
H	-3.6548041462	-2.41899631	-0.7203169813
H	-2.6282996115	-2.7368286505	-2.1270519527
H	-2.0693074827	-3.1791348701	-0.5038731622
H	-2.0693074827	-3.1791348701	-0.5038731622

TS 6-31++G(d,p) 0048

E(UwB97XD) = -1036.74629280 A.U.

First frequency = -1478.5027 cm⁻¹

S	-0.1984707244	1.1807405155	0.364435835
O	-0.2088337832	1.0827255283	1.8288625762
O	-1.1360130687	2.1146688889	-0.2704525166
N	-0.452402509	-0.3161011719	-0.3015687675
C	-1.5363647155	-0.5226884094	-1.2679719553
H	-1.7784462539	0.443869131	-1.7145926092
H	-1.133973498	-1.1630419813	-2.063721756
C	-2.8115978373	-1.1616275561	-0.6983185029
H	-2.5554929578	-2.160237629	-0.3196425781
C	0.0108235401	-1.5160915568	0.4154151025
H	-0.059530116	-2.3228488144	-0.3209488005
H	-0.6744419838	-1.765075556	1.23500078
C	1.4400113344	-1.4621450717	0.9646380154
H	1.7096544116	-2.4927697372	1.2368364766
H	1.4574416941	-0.8840896175	1.8941154483
C	2.4865952909	-0.8989324229	0.0179622551
H	2.0763300794	0.3129507402	-0.1140499534
C	3.8595141946	-0.7800745591	0.6477272557

H	4.5486988815	-0.235970993	-0.0056492534
H	4.2863392856	-1.7766967077	0.8269520632
H	3.8131850967	-0.2601956885	1.610135354
C	2.488223373	-1.4812219879	-1.3803799975
H	1.5160548102	-1.3644516325	-1.8687053481
H	2.7240035199	-2.554129491	-1.3475996268
H	3.2420874799	-0.9930333532	-2.0054859386
C	1.4491568304	1.5659472035	-0.1537465116
H	1.4273966568	1.7812625828	-1.2227809846
C	2.2233354122	2.5189784454	0.7161927901
H	2.2550972114	2.16770076	1.7504248376
H	1.7905819714	3.5263010995	0.7083993111
H	3.2479816359	2.5911077829	0.3414934388
C	-3.8229191196	-1.3391185484	-1.8335952684
H	-3.4056118281	-1.9326073817	-2.6542077089
H	-4.7236785441	-1.846616611	-1.4753683798
H	-4.1247040127	-0.3659006013	-2.2389702659
C	-3.4034761151	-0.3486368052	0.452409509
H	-3.6764108645	0.6577019908	0.1161137171
H	-4.3033359427	-0.8354614461	0.8414770872
H	-2.6948630715	-0.2429072596	1.2801439473
H	-2.6948630715	-0.2429072596	1.2801439473

TS 6-31++G(d,p) 0056

E(UwB97XD) = -1036.74710434 A.U.

First frequency = -1479.3553 cm⁻¹

S	-0.1839779647	1.3608017172	0.6013398645
O	0.4139413646	1.6198622821	1.9174144334
O	-1.3110319593	2.2067039063	0.1884887
N	-0.6801967175	-0.2255532771	0.4865412758
C	-2.1153641359	-0.512876439	0.3476108764
H	-2.464792128	-1.0005455085	1.2675870742
H	-2.6573766657	0.4302012884	0.2522573527
C	-2.4182698403	-1.3927968836	-0.8706513875
H	-1.8008496995	-2.2996685486	-0.8057006295
C	0.0620020145	-1.2440936792	1.2555651321
H	-0.2943730093	-2.2019249605	0.8666785884

H	-0.2251253192	-1.1959914254	2.3143482515
C	1.5890295358	-1.1983400705	1.1486564945
H	1.9608840487	-2.1489645927	1.5569174077
H	1.9804638315	-0.4098751959	1.7992261454
C	2.1461593964	-0.997264189	-0.2508387979
H	1.681644228	0.1685028349	-0.5314539883
C	3.6518122086	-0.8279683312	-0.2757436684
H	4.0011001767	-0.5437149766	-1.2733302558
H	4.1468164842	-1.7708402801	-0.0049324642
H	3.9802892954	-0.0637578821	0.4360279415
C	1.6101061986	-1.9342686372	-1.3127286444
H	1.9991777601	-1.6697003992	-2.3007677258
H	0.5182563025	-1.9123236991	-1.3609691742
H	1.9181803167	-2.9670258878	-1.0972452784
C	1.0920066892	1.4397137928	-0.6211814126
H	0.6232579646	1.4138524351	-1.6053412506
C	2.1603737971	2.4775752844	-0.4068932543
H	2.6208672873	2.3697518655	0.5781213738
H	1.7655724512	3.496713156	-0.492309974
H	2.934719981	2.3528936665	-1.1686435572
C	-2.0792817459	-0.6688279598	-2.1734765288
H	-2.2494551119	-1.3194521906	-3.0370529948
H	-2.7044192544	0.2242219838	-2.2916040231
H	-1.0320367684	-0.35271946	-2.1898104812
C	-3.887150052	-1.8202017101	-0.8364101262
H	-4.1251289333	-2.461189295	-1.6907032179
H	-4.1217761081	-2.3746140309	0.0783168837
H	-4.5463944361	-0.9449493022	-0.8802726329
H	-4.5463944361	-0.9449493022	-0.8802726329

TS 6-31++G(d,p) 0057

E(UwB97XD) = -1036.74664644 A.U.

First frequency = -1413.5217 cm⁻¹

S	0.0128165588	1.4627819953	-0.5861396184
O	-1.0573731221	2.3473887432	-0.1105080031
O	0.5755568616	1.724408858	-1.9180211258
N	-0.5664811222	-0.1098904436	-0.4907062679

C	-2.0302131496	-0.2835092392	-0.5012286477
H	-2.495626506	0.6733998735	-0.2578537357
H	-2.3503804237	-0.5580936416	-1.5165552281
C	-2.5152456056	-1.3365424761	0.5027533372
H	-1.9797519732	-2.2776054862	0.3188772126
C	0.1228662074	-1.1257644083	-1.3171892817
H	-0.1743812279	-1.0111221632	-2.3683246935
H	-0.2764903281	-2.0825106761	-0.9715808173
C	1.6517538643	-1.1670302675	-1.2371267645
H	2.0763409518	-0.3890565409	-1.879536347
H	1.9612350426	-2.1285344365	-1.6707572505
C	2.2457571356	-1.0245426027	0.1538055237
H	1.8769330924	0.1664712533	0.4359758016
C	1.6590460912	-1.9291339102	1.216809592
H	1.9013868608	-2.9781422836	0.9955806435
H	0.5709269791	-1.8399668342	1.2697956822
H	2.0703269973	-1.6935078487	2.2031956528
C	3.7597125615	-0.9640525135	0.1558314711
H	4.1296609212	-0.2155408683	-0.5522300706
H	4.1810817045	-1.9363777133	-0.1337686407
H	4.1433268388	-0.7181900574	1.1510223137
C	1.3471856071	1.4632864582	0.5733332629
H	2.1279667701	2.1290094137	0.2059385925
C	0.9710381658	1.5886306819	2.0245071
H	1.8660119301	1.451419994	2.6374981856
H	0.2401605325	0.8290117197	2.3115642318
H	0.5483146537	2.5731924804	2.2491884899
C	-4.0062465798	-1.5938711669	0.2697206739
H	-4.1984611625	-1.9423972098	-0.750350191
H	-4.3811817422	-2.352910902	0.9628796493
H	-4.5872221348	-0.6776024167	0.4295942596
C	-2.248781202	-0.9045062082	1.9438123846
H	-2.5955802973	-1.6662885299	2.6490942885
H	-1.1817990694	-0.7453091835	2.1173474039
H	-2.7716829268	0.0325353771	2.1698632521
H	-2.7716829268	0.0325353771	2.1698632521

TS 6-31++G(d,p) 0058

E(UwB97XD) = -1036.74524745 A.U.

First frequency = -1495.7227 cm⁻¹

S	0.0030356479	1.0882067806	-0.9875625658
O	-1.0246964756	2.0957310929	-0.7055945635
O	0.3208546297	0.7737587128	-2.3838675839
N	-0.4614951082	-0.3053797669	-0.2387455642
C	-1.4993132926	-0.2608672284	0.7983076351
H	-1.2828645203	-1.0832360953	1.4921215747
H	-1.3907949004	0.6679511065	1.3646052741
C	-2.9475030798	-0.3735236816	0.3053890952
H	-3.1419004344	0.49984822	-0.3281697574
C	0.0982288348	-1.6007522131	-0.6640548416
H	-0.3945520448	-1.9514845279	-1.5766890883
H	-0.1721942843	-2.2985654387	0.1323889329
C	1.6165843492	-1.6461957038	-0.8882361865
H	1.8535884544	-1.2343908151	-1.8738965681
H	1.8940593602	-2.7099539736	-0.923532916
C	2.4688748708	-0.9392422304	0.1514947422
H	2.1049404717	0.2891069601	-0.0041763789
C	2.1662001382	-1.2873633398	1.5943413161
H	2.3888388426	-2.3469502049	1.7833015298
H	1.1152200203	-1.118321214	1.846098595
H	2.777618432	-0.6912268813	2.2786002685
C	3.9457677886	-0.9355012411	-0.1875972879
H	4.1190139512	-0.5755581967	-1.2067737574
H	4.3577354597	-1.9515415718	-0.1163446097
H	4.5077354865	-0.2994384589	0.50362685
C	1.5166702886	1.5477627111	-0.1915785794
H	2.1529584566	2.0838090033	-0.8957107663
C	1.3861294419	2.131317042	1.1908125824
H	2.3839764145	2.2766816142	1.6133089718
H	0.83510456	1.4611268854	1.8572505596
H	0.8744577567	3.0991901407	1.1768715945
C	-3.8846769058	-0.3157711463	1.5144894708
H	-3.7227887818	-1.176973847	2.1747132136
H	-3.7265552228	0.5949772385	2.1019076586
H	-4.9309987516	-0.3325872068	1.1950050492

C	-3.1912220882	-1.6365340021	-0.521075688
H	-2.9250849045	-2.5365100262	0.0475592868
H	-4.2475906466	-1.7150626142	-0.7970012349
H	-2.6078789143	-1.630379837	-1.4458029834
H	-2.6078789143	-1.630379837	-1.4458029834

TS 6-31++G(d,p) 0059

E(UwB97XD) = -1036.74465785 A.U.

First frequency = -1515.0153 cm⁻¹

S	-0.166066787	1.0610418935	0.9258385628
O	0.1728478181	0.7821982866	2.324083864
O	-1.2399816023	2.0194456307	0.6414647425
N	-0.5744323153	-0.363803903	0.2110138036
C	-1.4821046029	-0.3478591375	-0.9422881665
H	-1.3347184008	0.5806958311	-1.502390291
H	-1.1749240159	-1.1674794572	-1.6035123043
C	-2.9680281095	-0.5001926505	-0.5977198138
H	-3.2443938599	0.3610169124	0.0218928238
C	0.055524608	-1.6236591418	0.6456778647
H	-0.1838917565	-2.3446651676	-0.1395810418
H	-0.4191151075	-1.9841348197	1.5641041469
C	1.5753514216	-1.5878341384	0.865987905
H	1.9061081512	-2.6348485324	0.9321240343
H	1.7906515449	-1.1355800126	1.8389335002
C	2.3921711718	-0.8696306568	-0.1949801527
H	1.9433916773	0.3398522944	-0.1098257745
C	3.860729111	-0.7552820646	0.1619154353
H	4.3382097103	-1.7448073544	0.1415010977
H	3.995922673	-0.3413291589	1.1663497253
H	4.3919418481	-0.115288299	-0.5495393618
C	2.1345813834	-1.2967091763	-1.625279122
H	2.4082765817	-2.3519571097	-1.7635601557
H	2.7312368679	-0.7026962208	-2.3242693278
H	1.0828552487	-1.1864178414	-1.9041561264
C	1.3090115552	1.5729376946	0.0886786532
H	1.0445537476	1.8758652666	-0.9256710806
C	2.2357319742	2.4882283406	0.8434071752

H	3.147523757	2.6360546436	0.2584298063
H	2.5085316714	2.0582614397	1.8101286916
H	1.7853773644	3.4722846491	1.0190455216
C	-3.2457572235	-1.7788603067	0.1929821312
H	-2.7227714214	-1.7769344478	1.1535416936
H	-4.3163722551	-1.8799235786	0.3969591962
H	-2.9260117085	-2.6649784801	-0.370005033
C	-3.7876168868	-0.4570517936	-1.889414015
H	-4.8583447417	-0.5133004472	-1.6713166635
H	-3.6060870897	0.4667685312	-2.4490377613
H	-3.5344544309	-1.3028872059	-2.5407254543
H	-3.5344544309	-1.3028872059	-2.5407254543

TS 6-31++G(d,p) 0061

E(UwB97XD) = -1036.74629278 A.U.

First frequency = -1478.6151 cm⁻¹

S	-0.2974256454	1.1568261875	0.413559842
O	-0.27649988	0.9707362022	1.8693039522
O	-1.2881554996	2.0823019694	-0.1487929698
N	-0.4948097093	-0.3076279304	-0.3381230303
C	-1.585499668	-0.5062264735	-1.2986083825
H	-1.8797254184	0.4730400217	-1.6817126341
H	-1.1686518145	-1.0779555873	-2.1379914665
C	-2.8195205119	-1.2374167728	-0.7494988922
H	-2.5110374525	-2.2439136875	-0.4364322901
C	0.0359000235	-1.5254548112	0.2973336
H	-0.0108473954	-2.2889278333	-0.4855893899
H	-0.6221029927	-1.8550426818	1.110779913
C	1.4710381766	-1.4377389303	0.8262980423
H	1.7925785422	-2.4690688729	1.0311188891
H	1.4792223891	-0.9162782347	1.7887967571
C	2.4730092563	-0.7702882075	-0.1006910219
H	2.0052787556	0.4268882773	-0.152241354
C	3.8504448574	-0.6252686656	0.5135356854
H	4.501788436	-0.0112234555	-0.1162480276
H	4.3257194915	-1.6097626492	0.6250778187
H	3.798149322	-0.1668638429	1.5064006855

C	2.4755060286	-1.2668245557	-1.5317237235
H	3.1943297197	-0.7069828546	-2.137749901
H	1.4901033255	-1.1668980271	-1.9966976069
H	2.7610710717	-2.3274534934	-1.5680011236
C	1.3211108189	1.649103554	-0.1057496537
H	1.2698305951	1.9272339802	-1.1591689078
C	2.0667552047	2.5831601904	0.8085824272
H	3.0799193357	2.7257150094	0.4229960452
H	2.1336790548	2.1720143689	1.8187909169
H	1.5882210174	3.5677255961	0.8691511268
C	-3.8421116386	-1.3934397246	-1.8778141529
H	-4.7116303675	-1.9639353276	-1.5376386657
H	-4.1961169256	-0.412821463	-2.217846379
H	-3.4127858348	-1.915524119	-2.7397237415
C	-3.4270894471	-0.5238854781	0.4576425772
H	-2.7091652804	-0.4350994398	1.2793207107
H	-3.7520029058	0.4869652488	0.1876074213
H	-4.2964485042	-1.0749420923	0.8300315108
H	-4.2964485042	-1.0749420923	0.8300315108

TS 6-31++G(d,p) 0064

E(UwB97XD) = -1036.74664633 A.U.

First frequency = -1413.8272 cm⁻¹

S	-0.0333876021	1.3726049293	-1.0379781893
O	-1.1286877422	2.2882104491	-0.6973398739
O	0.5032778607	1.4262678753	-2.4047746157
N	-0.5547896204	-0.1802960227	-0.6709809396
C	-2.0114524514	-0.4015222026	-0.6260229169
H	-2.5074934863	0.566661777	-0.5361749329
H	-2.3343334868	-0.8515596196	-1.5757645328
C	-2.446125931	-1.2881856132	0.5474480587
H	-1.8795656658	-2.2283764466	0.5128935305
C	0.1599494057	-1.2969670312	-1.3286627556
H	-0.1543129404	-1.3698260872	-2.3785841123
H	-0.2006548255	-2.1950213025	-0.82101362
C	1.6902359891	-1.2733842943	-1.2710218676
H	2.0785179537	-0.6004058779	-2.0420714836

H	2.0285219062	-2.2831266277	-1.5435979339
C	2.2963061477	-0.8803395927	0.0654124195
H	1.8885342562	0.3281197006	0.1519689371
C	1.7559076615	-1.6133849969	1.2750037632
H	2.0336136422	-2.6758033022	1.227758926
H	0.6659760465	-1.553500366	1.331954463
H	2.1702564317	-1.2020154578	2.200597383
C	3.8070140266	-0.7700239113	0.0293008782
H	4.1941782131	-0.3487025549	0.9623628742
H	4.1408209878	-0.138458388	-0.8002666428
H	4.2592990714	-1.7625022071	-0.1020790723
C	1.3141231314	1.611519498	0.0809365319
H	2.0660720321	2.2319103791	-0.4063765735
C	0.9514523151	1.9653471315	1.4973975349
H	0.2515988119	1.2407395192	1.9201965361
H	0.496735886	2.9591112674	1.5622592976
H	1.8581185671	1.9622779824	2.1085506471
C	-3.9296883411	-1.6302746963	0.3874452668
H	-4.2681024325	-2.2768040753	1.2027151832
H	-4.5413058136	-0.7201979291	0.4053074875
H	-4.1221408377	-2.1484574455	-0.5577596051
C	-2.1776481214	-0.6134003798	1.8916603107
H	-2.732061902	0.3295947675	1.9688352991
H	-2.4869733235	-1.2586486425	2.7198978907
H	-1.1151869352	-0.3908240562	2.0163890704
H	-1.1151869352	-0.3908240562	2.0163890704

TS 6-31++G(d,p) 0065

E(UwB97XD) = -1036.74588972 A.U.

First frequency = -1415.1478 cm⁻¹

S	-0.0521749411	1.3891538074	-0.354116491
O	-1.1505683294	2.181129758	0.2123010688
O	0.5293443117	1.8487506351	-1.6224671682
N	-0.6096145098	-0.1814257208	-0.473760559
C	-2.0782319534	-0.3481457227	-0.4329371889
H	-2.5749025996	0.5179842388	-0.8800465986
H	-2.311257135	-1.2086337765	-1.0698615323

C	-2.6280796604	-0.5964974905	0.9735382678
H	-2.3000019289	0.2370623391	1.6060771174
C	0.0770399071	-1.1215705899	-1.3896886718
H	-0.3285682845	-1.0095516903	-2.4039077509
H	-0.209049514	-2.1152847972	-1.0312849094
C	1.6039902536	-1.038885113	-1.4770069106
H	1.8911692225	-0.1717527281	-2.0780067134
H	1.9209606256	-1.9270241859	-2.0428653658
C	2.3630632715	-0.9952563385	-0.1608703722
H	1.9168842715	0.0872511951	0.359098938
C	2.0354074555	-2.099282135	0.8217775707
H	2.3529226429	-3.0713985831	0.419378463
H	0.9632812763	-2.1574580004	1.0247853546
H	2.5536915247	-1.9461137002	1.7732416394
C	3.8472767168	-0.7462267008	-0.3384324037
H	4.0312486735	0.1344061184	-0.9620131797
H	4.3236059811	-1.6079570424	-0.8258695218
H	4.3402477595	-0.5955557332	0.6270778856
C	1.2557476484	1.2403398705	0.8203402087
H	1.9612324016	2.0582533613	0.673668597
C	0.8362089898	0.9373651855	2.2331131536
H	1.7242464085	0.7276169188	2.835392563
H	0.1835696618	0.0602753183	2.267407781
H	0.3053961695	1.7806603273	2.6874349864
C	-2.0942889318	-1.9016332772	1.5618605225
H	-1.001192313	-1.9033964414	1.5916900696
H	-2.4580478305	-2.0484569923	2.5836655166
H	-2.4182927505	-2.7603797949	0.9607474753
C	-4.1575049135	-0.5944843021	0.9288936813
H	-4.5444298338	0.3583129701	0.5528508593
H	-4.5296655895	-1.3932005798	0.2753874175
H	-4.5752819109	-0.7588187873	1.9268656855
H	-4.5752819109	-0.7588187873	1.9268656855

TS 6-31++G(d,p) 0068

E(UwB97XD) = -1036.74050994 A.U.

First frequency = -1405.3582 cm^{-1}

S	-0.100724124	1.1742614129	0.2549433887
O	0.3251778864	1.1202741513	1.6638991299
O	-1.1042567006	2.2032298301	-0.0527122247
N	-0.7263449311	-0.2833743658	-0.2663279008
C	-1.9503940981	-0.6741239627	0.4576724071
H	-1.6999056859	-1.4262166679	1.2181110769
H	-2.3420255627	0.200192897	0.9872584924
C	-3.0416008021	-1.2003282989	-0.4813626346
H	-2.6282953162	-2.0397321613	-1.0566409656
C	0.1772108842	-1.3985603396	-0.6168198628
H	0.5894114362	-1.214002476	-1.6141275853
H	-0.4796257706	-2.2639488144	-0.7184802504
C	1.3091347604	-1.7173643836	0.3743334802
H	1.5610989242	-2.781671441	0.2752769613
H	0.9458708244	-1.5681009974	1.3964564743
C	2.5682828307	-0.889527355	0.1256494232
H	2.0783932902	0.2102692777	-0.3061383458
C	3.3550271123	-0.5370349123	1.3692430078
H	4.201861379	0.1146735994	1.1313670412
H	3.7563005891	-1.4479070783	1.8352564551
H	2.7182816166	-0.0327136726	2.1015520141
C	3.4171886147	-1.3857510742	-1.029507929
H	3.8988582612	-2.335740146	-0.7610195026
H	4.2058598554	-0.6680748997	-1.2757454212
H	2.8221507961	-1.5599294852	-1.9319490936
C	1.3427365644	1.3392685044	-0.7383767278
H	1.1039410437	1.1838172889	-1.7904827757
C	2.1914709795	2.5398138253	-0.4073653178
H	3.1186842237	2.4844216468	-0.9832299476
H	2.445001336	2.5604574284	0.6554407017
H	1.688910705	3.4787108406	-0.6650147354
C	-3.4969016269	-0.1220630626	-1.4636748028
H	-2.6522464162	0.268761277	-2.0373898737
H	-4.2362652751	-0.5238258596	-2.1637130657
H	-3.956345364	0.716816523	-0.9277550414
C	-4.2106833086	-1.7312842797	0.351389069
H	-3.8913933689	-2.5304335712	1.0286440946
H	-4.6513288484	-0.9299663305	0.9565706155

H -4.996574779 -2.1309662608 -0.2965614532
H -4.996574779 -2.1309662608 -0.2965614532

TS 6-31++G(d,p) 0069

E(UwB97XD) = -1036.74418391 A.U.

First frequency = -1461.1820 cm^{-1}

S -0.1274725755 1.3129248968 0.224994236
O 0.401682019 1.8118285021 1.5015671605
O -1.172891844 2.1146565389 -0.4232785981
N -0.7261500681 -0.2373695212 0.3798412761
C -2.1918556591 -0.3857442224 0.2583817085
H -2.4508082456 -1.2803513466 0.8348331985
H -2.7103028024 0.4544664555 0.732486164
C -2.6875976619 -0.5635780411 -1.1797627826
H -2.4494065771 0.3529372253 -1.7307713486
C -0.1095478077 -1.1305803087 1.3877890923
H -0.4340806692 -2.1351819027 1.1017577422
H -0.5294961528 -0.9195093763 2.3801783353
C 1.4183154624 -1.1108921668 1.4936663602
H 1.6903589032 -1.9666549925 2.1284897726
H 1.7397825207 -0.2143378183 2.0311622686
C 2.1833875262 -1.1988186121 0.1834069459
H 1.7727950674 -0.1400428732 -0.419532683
C 3.6751944369 -0.9894911379 0.3494200414
H 4.17692373 -0.9321904812 -0.6216345088
H 4.1186038639 -1.8274085896 0.9050547155
H 3.8908912009 -0.0710373351 0.9046662795
C 1.8208797837 -2.366422478 -0.7095013248
H 0.7451099386 -2.4220619442 -0.8925993936
H 2.1308104797 -3.3104531525 -0.2397572324
H 2.3282865517 -2.29364797 -1.6764205967
C 1.2220914019 1.0646020272 -0.8868988866
H 0.8158641137 0.7803880802 -1.8583129491
C 2.2961389788 2.1185953628 -0.8769558173
H 1.9298841113 3.0802322272 -1.2550653049
H 3.1180289081 1.7960623029 -1.5216980622
H 2.6859531088 2.2722717434 0.1322767743

C	-4.2084559579	-0.7340923976	-1.1633935915
H	-4.7017770853	0.1160017041	-0.6802940749
H	-4.600137405	-0.8161189085	-2.1818373325
H	-4.4936691115	-1.6441467463	-0.6209970857
C	-2.0020700535	-1.7397599982	-1.8732865149
H	-0.9235605054	-1.5763047678	-1.9446163759
H	-2.1712260082	-2.6735849814	-1.3218856487
H	-2.3920820417	-1.8726665853	-2.8874384655
H	-2.3920820417	-1.8726665853	-2.8874384655

TS 6-31++G(d,p) 0079

E(UwB97XD) = -1036.74710429 A.U.

First frequency = -1479.2511 cm⁻¹

S	-0.2407419058	1.3029400359	0.8688929233
O	0.3796436817	1.3932717691	2.1969140009
O	-1.4010981466	2.1620296415	0.6009716377
N	-0.6932285776	-0.2665755173	0.5402918536
C	-2.1223904204	-0.5771601109	0.3897538672
H	-2.4359268664	-1.2001612017	1.2381893116
H	-2.6934981647	0.3521866424	0.4388782916
C	-2.4282439415	-1.2863128433	-0.9345292226
H	-1.7835060134	-2.173125494	-1.0101440027
C	0.0957396862	-1.3589044215	1.1436963796
H	-0.2418130396	-2.2634988308	0.6304370976
H	-0.1679579236	-1.4690996982	2.2039345708
C	1.6179190279	-1.249905955	1.015497864
H	2.0265119054	-2.2361507309	1.2782013685
H	2.001330022	-0.5487377052	1.7634927709
C	2.1364187199	-0.836201249	-0.3517724324
H	1.6318880794	0.3419469569	-0.4560257302
C	3.6355362378	-0.6169665744	-0.3809333104
H	4.1638657251	-1.5723533442	-0.2565268549
H	3.9582527775	0.0488523242	0.4259543769
H	3.9530276082	-0.1832410044	-1.3343860964
C	1.6033142477	-1.6311530857	-1.5251376432
H	1.9466776706	-2.6734046477	-1.4639627663
H	1.9610408152	-1.2175221006	-2.4730520039

H	0.5104589375	-1.6381068635	-1.5488427415
C	1.0038061553	1.5937489147	-0.3539923975
H	0.5133299162	1.6918153257	-1.3228974014
C	2.0464836835	2.624548874	-0.0152327585
H	1.6205232275	3.6324180081	0.0523213646
H	2.8059802348	2.633410437	-0.8016829324
H	2.5329360934	2.3935319008	0.9355210676
C	-2.1410104507	-0.3759102255	-2.1282904653
H	-2.7940276049	0.5046580945	-2.1068529392
H	-1.1039068107	-0.0276808418	-2.1200942985
H	-2.3129373348	-0.9036233469	-3.0716857739
C	-3.882948425	-1.7609599042	-0.9328217814
H	-4.0797625571	-2.4460690669	-0.1015358822
H	-4.5680480849	-0.9097750133	-0.8394471254
H	-4.1224596876	-2.2822933156	-1.8645737648
H	-4.1224596876	-2.2822933156	-1.8645737648

TS 6-31++G(d,p) 0081

E(UwB97XD) = -1036.74282345 A.U.

First frequency = -1427.9908 cm^{-1}

S	0.0672619516	1.0084948521	-0.8475309202
O	-0.9518609629	2.0632669139	-0.7964032312
O	0.5681339247	0.6123808885	-2.1668452279
N	-0.5944411654	-0.3060767472	-0.092279517
C	-1.8426521552	-0.1238924214	0.6663762235
H	-1.7925057659	-0.8075897525	1.5231329693
H	-1.8893941463	0.8916129187	1.0679609363
C	-3.1085194078	-0.4095193109	-0.1486288108
H	-3.1329651926	0.3167167762	-0.9703751166
C	0.1946124141	-1.4987417669	0.2870273926
H	-0.4808978682	-2.3491042092	0.1626531395
H	0.4296062758	-1.434182753	1.3589987316
C	1.4735646543	-1.783017454	-0.5022057562
H	1.2702388266	-1.69514244	-1.5723973419
H	1.7247721079	-2.8356328941	-0.3106820271
C	2.6846586041	-0.9335154374	-0.1242023089
H	2.2032716384	0.2496150339	-0.0007055215

C	3.2751097346	-1.2401509148	1.2391467957
H	4.0490754635	-0.5127322729	1.5028057138
H	3.7390102049	-2.2360846953	1.2338039262
H	2.5203029277	-1.23040078	2.0314563732
C	3.7132208624	-0.8217157364	-1.229642717
H	4.5330513322	-0.1555527188	-0.9429708632
H	3.2570326724	-0.4408618395	-2.1481503057
H	4.1454297541	-1.8079881784	-1.4489156079
C	1.4797183429	1.4512120733	0.1118648565
H	2.0798253403	2.1713980643	-0.444958677
C	1.234664048	1.7425032167	1.5677228475
H	2.1927997614	1.8725108608	2.0773697495
H	0.7001090875	0.9228591944	2.0577060107
H	0.6504198755	2.6595775943	1.7037493856
C	-4.3380784559	-0.1853518751	0.7339179911
H	-4.346662464	-0.8882288475	1.5762686805
H	-4.3587213657	0.8310776001	1.1412566459
H	-5.2588918302	-0.338258627	0.1628525076
C	-3.1010043443	-1.816164678	-0.746958776
H	-4.0063521208	-1.989440777	-1.3371935482
H	-2.2385622732	-1.9617128071	-1.4047710539
H	-3.0654332372	-2.5765090218	0.0436902797
H	-3.0654332372	-2.5765090218	0.0436902797

TS 6-31++G(d,p) 0082

E(UwB97XD) = -1036.74021243 A.U.

First frequency = -1420.0817 cm⁻¹

S	-0.1505121748	1.1067786477	0.2145550864
O	0.1959165066	1.011138943	1.6361004982
O	-1.1181239264	2.1422467074	-0.166424968
N	-0.7707839154	-0.355332473	-0.2832001175
C	-1.9146560179	-0.3509706473	-1.2152619386
H	-2.041951304	0.6532376198	-1.6237134609
H	-1.6600050311	-1.0146425952	-2.0507916092
C	-3.2368661046	-0.8015459854	-0.5753369065
H	-3.9658005091	-0.7900440258	-1.3978111167
C	0.1214566992	-1.5280852154	-0.4393192406

H	0.5508469069	-1.5182630391	-1.4524966771
H	-0.5385478878	-2.3945312021	-0.3863373431
C	1.2369021442	-1.6992888453	0.5964122965
H	1.4876632298	-2.7683690024	0.6211383124
H	0.8565020965	-1.4375939898	1.587219748
C	2.5123296088	-0.9169339293	0.2879363694
H	2.0562570351	0.1725131966	-0.2083128329
C	3.3051047855	-0.5114491841	1.5117029926
H	4.1696642522	0.102235058	1.2389313689
H	3.6808782512	-1.4027771711	2.0336237622
H	2.6805519404	0.0520036139	2.2108247905
C	3.3541756082	-1.506503344	-0.8276699282
H	4.1632388358	-0.8261354401	-1.1111122399
H	2.76164778	-1.7200174336	-1.723029117
H	3.8094651848	-2.4501878522	-0.4973650139
C	1.3616348525	1.3047974793	-0.674429614
H	1.1901491822	1.1389715818	-1.7391449682
C	2.1932810529	2.503075493	-0.2981128825
H	1.7030590047	3.4424072926	-0.5777713151
H	3.1507490411	2.4525590286	-0.8234287156
H	2.3897219866	2.5210124259	0.7768572646
C	-3.7142980195	0.1777224846	0.497742387
H	-3.8064231171	1.1926503271	0.1006256485
H	-4.6880187196	-0.1305135803	0.8920259729
H	-3.0066286644	0.2086110125	1.3336432613
C	-3.1742875692	-2.2265183386	-0.021308329
H	-4.1594413657	-2.5401722342	0.338048881
H	-2.8512406009	-2.9442531178	-0.7836057001
H	-2.4810857457	-2.2838173783	0.8256934935
H	-2.4810857457	-2.2838173783	0.8256934935

TS 6-31++G(d,p) 0089

E(UwB97XD) = -1036.73838142 A.U.

First frequency = -1407.5751 cm^{-1}

S	-0.1620112313	1.097882556	0.4453917979
O	0.4051749198	0.9491174974	1.7968518639
O	-1.2090425863	2.1206389062	0.3213107181

N	-0.8046974965	-0.3358682388	-0.1229642306
C	-1.9751879955	-0.7919340526	0.6585855246
H	-1.7069591686	-1.7221285882	1.1745367916
H	-2.1934701974	-0.0555614308	1.4375599495
C	-3.2434594547	-0.9917366213	-0.1847186257
H	-3.99755053	-1.3533105242	0.5282240384
C	0.102332239	-1.3993739807	-0.6104635248
H	0.4104904201	-1.1506914908	-1.6316053483
H	-0.5279196971	-2.2837544058	-0.693003017
C	1.3339424238	-1.7265802071	0.2510744517
H	1.6047301369	-2.7751110498	0.0680992023
H	1.0662615149	-1.6445778345	1.3093517867
C	2.5412467573	-0.8473563137	-0.0677729954
H	1.9828179981	0.2571815233	-0.3850224457
C	3.4347437828	-0.5400742788	1.1141930637
H	3.9006742503	-1.4626730758	1.4878734757
H	2.8582654758	-0.0953528221	1.9302405837
H	4.2389143832	0.1483439735	0.8351190478
C	3.2876012219	-1.253072702	-1.3246464619
H	4.0294804749	-0.4984388742	-1.603669749
H	2.6130857778	-1.3974107204	-2.1749475629
H	3.8181115081	-2.2003195331	-1.1573576281
C	1.1706747779	1.3800501997	-0.6696108025
H	0.8350389712	1.2797210403	-1.7017452013
C	2.0076271306	2.5904158853	-0.3440715414
H	2.3644744568	2.5557133173	0.6883240871
H	1.4511343616	3.5228924075	-0.4899460585
H	2.8749194857	2.6076112271	-1.0088941807
C	-3.0872745039	-2.054922397	-1.2745915194
H	-4.0465966699	-2.2294216118	-1.7716858444
H	-2.3740263485	-1.7311932579	-2.0409683785
H	-2.7451376704	-3.0117167615	-0.8646504744
C	-3.7404044305	0.3265136093	-0.7785344152
H	-4.6699401713	0.1695545133	-1.3352303959
H	-3.9259242662	1.0708841424	0.0012618444
H	-2.994438492	0.7434512195	-1.462612017
H	-2.994438492	0.7434512195	-1.462612017

TS 6-311++G(d,p) 0003

E(UwB97XD) = -1036.89724316 A.U.

First frequency = -1515.0694 cm⁻¹

S	-0.1109804753	1.4343778104	0.6142091209
O	0.443834482	1.4734291108	1.9623626322
O	-1.131853048	2.4148170099	0.257134946
N	-0.7871558557	-0.0681627971	0.4086071765
C	-1.5083943459	-0.2871274879	-0.8532302931
H	-1.9798270572	0.6587257887	-1.1268361121
H	-0.814490902	-0.5590515331	-1.6603294265
C	-2.5978598295	-1.3562476562	-0.737103247
H	-2.123565525	-2.3188529069	-0.5123300657
C	-0.0661230641	-1.2171823881	0.9786653691
H	-0.8198082339	-1.9685931303	1.2227077377
H	0.3625596522	-0.895686911	1.9271661463
C	1.0006728165	-1.8401106101	0.0721804505
H	0.5450850204	-2.1349961051	-0.8783438522
H	1.3283738096	-2.7729269394	0.5513728187
C	2.2221622818	-0.9718535759	-0.1895390321
H	1.7479697426	0.2134503449	-0.4141199654
C	3.1198406785	-0.7703014655	1.0141584374
H	3.9284357403	-0.0706931374	0.7864262248
H	3.5761083162	-1.7236264786	1.3098006915
H	2.5691863968	-0.3782261521	1.8726783045
C	2.9639592357	-1.3255979766	-1.4601253844
H	2.2949346337	-1.3222887173	-2.3253998268
H	3.4009267458	-2.3294452555	-1.3802773403
H	3.7801744668	-0.6236158298	-1.6512178803
C	1.2259224647	1.5088005283	-0.5387590831
H	0.8210361773	1.5324680594	-1.5499321037
C	2.3250743346	2.4884271062	-0.2316268282
H	1.9848614191	3.5247950997	-0.326936717
H	3.1461497584	2.339238753	-0.9364369602
H	2.7061104076	2.3427022855	0.7805773679
C	-3.297147598	-1.492754594	-2.0898966555
H	-4.0514157756	-2.2827575115	-2.0557063343
H	-3.8007451705	-0.5590549599	-2.3619654225

H	-2.5870927755	-1.7386674426	-2.8848504289
C	-3.5902819968	-1.0265311173	0.3749850603
H	-4.3618740154	-1.7978910542	0.4438527778
H	-3.0944799377	-0.9483340165	1.3451569541
H	-4.08375702	-0.0693835767	0.1750009266
H	-4.08375702	-0.0693835767	0.1750009266

TS 6-311++G(d,p) 0023

E(UwB97XD) = -1036.89639366 A.U.

First frequency = -1506.6817 cm⁻¹

S	-0.1350977719	1.384679524	0.6935591243
O	0.7225117068	1.6255779118	1.8519519476
O	-1.2629391391	2.2870721811	0.4744682988
N	-0.7374687226	-0.1462525357	0.787133363
C	-2.1517485026	-0.4335538893	0.545135067
H	-2.5849982458	-0.8254208134	1.4733568408
H	-2.6531703046	0.5105921955	0.3283151495
C	-2.4091077665	-1.4205986997	-0.5981493716
H	-1.9207632646	-2.3713119174	-0.350680493
C	0.1197787597	-1.2115862172	1.3182831284
H	-0.5484333026	-1.9446895373	1.7760373446
H	0.7337660143	-0.8038842513	2.1238235595
C	0.9939932059	-1.904943082	0.2682268482
H	0.3536174279	-2.2972633825	-0.5262363903
H	1.4627114517	-2.7752622331	0.7493677634
C	2.0880826315	-1.0399008902	-0.3384287224
H	1.5134232352	0.0952701686	-0.5811422562
C	3.2081258653	-0.676663188	0.6148971761
H	2.8324011611	-0.2003387576	1.523761495
H	3.9151044617	0.0113650154	0.1437472454
H	3.7629808774	-1.5771407051	0.9078001809
C	2.5618089269	-1.5172034594	-1.6940257104
H	3.2853778416	-0.8220553236	-2.1283915645
H	1.7264888419	-1.6271802884	-2.3917020097
H	3.0520977656	-2.49538541	-1.6053982745
C	0.9058185513	1.349580848	-0.7304790128
H	0.2814816164	1.2367515539	-1.6152265987

C	1.9908499376	2.3882052638	-0.7982754546
H	1.5825309257	3.3965356732	-0.9236354509
H	2.6333535111	2.1790307878	-1.6567117029
H	2.6026632824	2.3743652048	0.1051897815
C	-1.8468682617	-0.914181154	-1.9239206708
H	-2.0710889225	-1.6142230457	-2.7330590551
H	-2.2854936904	0.0554968775	-2.1841712756
H	-0.7621349043	-0.7929707158	-1.8797411932
C	-3.9127411917	-1.6798633375	-0.6961571595
H	-4.4482103294	-0.7588078501	-0.9507080011
H	-4.1297040753	-2.4186713587	-1.471640634
H	-4.3162857899	-2.0541909451	0.2490864674
H	-4.3162857899	-2.0541909451	0.2490864674

TS 6-311++G(d,p) 0025

E(UwB97XD) = -1036.89584199 A.U.

First frequency = -1463.4222 cm⁻¹

S	0.0544237187	1.5110667337	-0.5900854986
O	-0.9886367786	2.4401256698	-0.1619312375
O	0.7161721036	1.7710713817	-1.8687504142
N	-0.6145682755	-0.0107138744	-0.581725913
C	-2.0748393141	-0.1552697379	-0.573550116
H	-2.5046995556	0.7723944076	-0.1944006915
H	-2.4367451273	-0.2936524645	-1.6008057223
C	-2.5483222096	-1.3202639448	0.3011090013
H	-2.087954401	-2.2449132134	-0.0690307549
C	0.1492772889	-1.0716309377	-1.2595277512
H	0.7319873244	-0.6413773829	-2.0781822288
H	-0.5788378051	-1.7408742903	-1.7209861435
C	1.0444529786	-1.8639544946	-0.3063129749
H	1.3934353858	-2.7626574096	-0.8336526435
H	0.4367379281	-2.2078002915	0.5354208559
C	2.2556015803	-1.0979519771	0.2034419063
H	1.823402897	0.0979225324	0.4119866078
C	2.759899475	-1.5649418616	1.5510640737
H	3.1469779149	-2.5896780544	1.4784256488
H	1.9602663079	-1.5646108789	2.2971421154

H	3.5724361353	-0.9292307583	1.9135014623
C	3.347410239	-0.8926283928	-0.8268636792
H	4.1254675652	-0.2259580815	-0.445448601
H	2.9595512664	-0.4604131638	-1.7528331394
H	3.8189641596	-1.8517723482	-1.0748097667
C	1.3224300626	1.3933842174	0.6281061315
H	2.1416380913	2.0507799728	0.3434733643
C	0.8733425561	1.4401740117	2.0613630306
H	1.7204134767	1.2132848671	2.7125498621
H	0.0877953674	0.7074412961	2.2539305239
H	0.4922299591	2.4295353333	2.3302673638
C	-4.0638029131	-1.4620691569	0.1557964863
H	-4.3531289609	-1.6179341375	-0.8874123115
H	-4.4309126575	-2.3106277177	0.7384829245
H	-4.5729459035	-0.561950903	0.5168975618
C	-2.1468788396	-1.1347810087	1.7618953919
H	-2.5189181939	-1.9612430894	2.3733218642
H	-1.0614802639	-1.0954400685	1.8731651394
H	-2.5620341708	-0.2031731749	2.1618188446
H	-2.5620341708	-0.2031731749	2.1618188446

TS 6-311++G(d,p) 0035

E(UwB97XD) = -1036.89667485 A.U.

First frequency = -1485.8178 cm⁻¹

S	0.1006644924	1.1498840885	-1.0097861109
O	-0.9101643096	2.1874723437	-0.8284534903
O	0.6107309115	0.8863586788	-2.3513021134
N	-0.5616061447	-0.2510218276	-0.4501519844
C	-1.5816408766	-0.1994252489	0.6056841991
H	-1.3989594181	-1.0468235872	1.2762407103
H	-1.4552126426	0.7058887226	1.2027684344
C	-3.0184313851	-0.2493645294	0.0783541174
H	-3.1576966416	0.6385372388	-0.5475346504
C	0.1425129456	-1.5178125411	-0.6836392519
H	0.5164673654	-1.515221841	-1.7080557492
H	-0.6149924211	-2.3012290496	-0.6332322462
C	1.2615744967	-1.8241710921	0.3167998038

H	1.5260924119	-2.8855352786	0.2084087251
H	0.8687131141	-1.7091616722	1.3331440064
C	2.5266353887	-0.9942875273	0.1606446491
H	2.1040171064	0.2216686465	0.0557549731
C	3.4011001836	-0.9847662539	1.3961241321
H	4.2417879382	-0.2952444457	1.2806756208
H	3.8145081557	-1.98541161	1.5775684502
H	2.8352114963	-0.6938298895	2.2855537217
C	3.2889950787	-1.2282877448	-1.1272777038
H	2.6611033289	-1.0829234682	-2.0090513969
H	3.6813170904	-2.2529703418	-1.1539256424
H	4.1376960507	-0.543794154	-1.2055680081
C	1.5061185621	1.488269526	0.0060121862
H	2.2009928186	2.1140496263	-0.5510790267
C	1.2346181785	1.8687167545	1.4361187993
H	0.7194193559	1.0677050204	1.9728363528
H	0.6278189802	2.7762899389	1.5082261883
H	2.1833107073	2.0519214944	1.9442821993
C	-3.9879712106	-0.1726957271	1.2573403066
H	-3.8708759936	-1.0414553169	1.9150450191
H	-3.8211489436	0.7282819125	1.8550726039
H	-5.0233144328	-0.1574059429	0.9074956561
C	-3.2790730535	-1.4886327755	-0.7745501013
H	-2.6171101939	-1.5208100303	-1.6435059808
H	-3.1265646215	-2.403707942	-0.1903398745
H	-4.3096473736	-1.4939227848	-1.1394705368
H	-4.3096473736	-1.4939227848	-1.1394705368

TS 6-311++G(d,p) 0036

E(UwB97XD) = -1036.89469504 A.U.

First frequency = -1431.0943 cm⁻¹

S	-0.0353268002	1.4141482949	-0.3320911407
O	-1.1244861997	2.2460307771	0.174193028
O	0.669611742	1.8685430849	-1.5301857975
N	-0.6619552261	-0.1057455946	-0.5729041229
C	-2.1272933314	-0.2547805405	-0.5240152537
H	-2.608507309	0.6589170368	-0.8782964924

H	-2.388208686	-1.0451334759	-1.2333250565
C	-2.6709732605	-0.6133644248	0.8601242337
H	-2.3421105708	0.1690259368	1.5532471709
C	0.1356093874	-1.03868421	-1.3898226459
H	0.5851231791	-0.503186692	-2.2309983154
H	-0.5693854167	-1.7526952319	-1.8148932801
C	1.198993892	-1.8124079274	-0.6074135901
H	1.5680822565	-2.6153575226	-1.2615147146
H	0.7186351246	-2.3020204778	0.2443242482
C	2.3929935601	-1.0034082774	-0.1259139749
H	1.8728067232	0.0537188305	0.3851744278
C	3.1410071158	-1.6506084018	1.0196183723
H	3.6171648385	-2.5817422957	0.6857795116
H	2.4686889089	-1.89947989	1.845476325
H	3.9283021627	-0.993921248	1.3997454004
C	3.2902220358	-0.47655475	-1.2268222681
H	3.7826724261	-1.3102714479	-1.7434369468
H	4.0706773615	0.170126038	-0.8170826521
H	2.7318894565	0.1004206544	-1.9671874252
C	1.1834436938	1.1611330931	0.9118891275
H	1.9015758455	1.9779189657	0.8670915834
C	0.6795431963	0.7570565186	2.2679666783
H	0.0929422981	1.5538391967	2.7354635549
H	1.5286446078	0.5347297546	2.9176811496
H	0.0549907113	-0.1367082619	2.2036049933
C	-2.1404599359	-1.9587976763	1.3476970264
H	-2.4440777844	-2.7641098126	0.669016523
H	-1.0497078248	-1.9615623293	1.4044667365
H	-2.5277417031	-2.1934759623	2.3428366375
C	-4.1990128574	-0.605237676	0.8186403767
H	-4.5729805178	-1.355497231	0.1128805523
H	-4.6155661659	-0.8372354183	1.8021458421
H	-4.5845513444	0.3705448275	0.5097758484
H	-4.5845513444	0.3705448275	0.5097758484

TS 6-311++G(d,p) 0038

E(UwB97XD) = -1036.89421591 A.U.

First frequency = -1475.7090 cm⁻¹

S	-0.1048522551	1.2558550617	-0.4605139182
O	-1.1148610955	2.1336452439	0.1247416835
O	0.059875058	1.2621971775	-1.9121334512
N	-0.4244523481	-0.2835828789	0.052608759
C	-1.5571100475	-0.5548352235	0.9404508025
H	-1.2006220284	-1.2440811147	1.7154675627
H	-1.832214323	0.3782596766	1.4336159823
C	-2.7903399595	-1.1538819541	0.2525858838
H	-2.5051242115	-2.1216314628	-0.1776943078
C	0.1032941445	-1.4362622835	-0.6944030137
H	-0.5171540682	-1.6401884879	-1.5739570886
H	-0.0157427281	-2.2845255285	-0.0147451193
C	1.5677751624	-1.3488863786	-1.1315598873
H	1.6510782716	-0.7253867343	-2.0249678953
H	1.8635874143	-2.3626469629	-1.4338933129
C	2.5371319094	-0.8350184764	-0.0829060022
H	2.1232862698	0.3729410941	0.0804847037
C	2.4370054944	-1.492745377	1.2760727201
H	2.6977570094	-2.5568885664	1.203122494
H	1.4274080271	-1.4232080224	1.688345118
H	3.1259451097	-1.0297409067	1.9872203849
C	3.9515143998	-0.6840532162	-0.5988757296
H	3.9759271991	-0.1110966265	-1.5299068485
H	4.3922909132	-1.66881758	-0.8005837192
H	4.5876761059	-0.1797910483	0.1335775267
C	1.4697291796	1.6025033328	0.2599864115
H	2.0029099397	2.3233211459	-0.3568037122
C	1.461453161	1.8335432365	1.7456870458
H	2.4897931069	1.8688108006	2.1124221157
H	0.9451170915	1.0225181074	2.2658818469
H	0.9726440461	2.7765692812	2.0065585895
C	-3.3103282947	-0.2619501676	-0.8718789971
H	-4.1848503249	-0.7145301502	-1.3471007655
H	-3.5994730344	0.7196735497	-0.484165924
H	-2.5530678055	-0.1039452949	-1.6447806946
C	-3.8678412176	-1.4100743354	1.3062653682
H	-4.7422208221	-1.8898339291	0.8592351565
H	-3.4997440858	-2.0591996244	2.1064258731

H -4.1970914919 -0.4686272186 1.7593141798
H -4.1970914919 -0.4686272186 1.7593141798

TS 6-311++G(d,p) 0039

E(UwB97XD) = -1036.89263160 A.U.

First frequency = -1506.6768 cm⁻¹

S -0.045972384 1.4366274004 0.7227689544
O 0.64113747 1.4161219548 2.0089863811
O -1.0675056302 2.4560263962 0.5020071689
N -0.7838074143 -0.0415211575 0.5417761767
C -1.6619785109 -0.1903482036 -0.629815037
H -2.0582502672 0.8019954203 -0.8417391175
H -1.0919092489 -0.5094626391 -1.5137599358
C -2.8410981568 -1.1546361436 -0.3924374173
H -3.0383875005 -1.1669076759 0.6850268356
C -0.0401979701 -1.2241984614 1.0029777915
H -0.7877524476 -1.9697653738 1.2784822963
H 0.4680019861 -0.9515873711 1.9271626323
C 0.9425129599 -1.823905526 -0.0087583272
H 0.4154562575 -2.0524347562 -0.9400898058
H 1.2749760657 -2.7905343692 0.3948512
C 2.1676296616 -0.9758423736 -0.3145368897
H 1.7002119586 0.2189332748 -0.4855806524
C 3.1378703109 -0.8238981664 0.8388600704
H 3.9530869893 -0.1444829508 0.5761563494
H 3.5809785004 -1.7958645319 1.0907809536
H 2.6501418065 -0.4312685242 1.7340203595
C 2.8272422796 -1.3130787976 -1.6341943028
H 2.1104456713 -1.2732397331 -2.4592696202
H 3.2448389866 -2.3278442622 -1.6040616147
H 3.6472016632 -0.6242161519 -1.8546089696
C 1.1718926028 1.516104713 -0.5540273295
H 0.6698895953 1.5471916743 -1.5206142987
C 2.3000922455 2.4891471798 -0.3480701721
H 1.9556311225 3.52752515 -0.3926781196
H 3.0434502578 2.3485536561 -1.1359619941
H 2.7831438635 2.3273608138 0.6171557914

C	-2.5506325825	-2.5821046286	-0.8655972341
H	-1.6837282657	-3.0258222613	-0.372194269
H	-3.4089623126	-3.2309171576	-0.6719343778
H	-2.3613526006	-2.5926681661	-1.9444500697
C	-4.0878270619	-0.6187131459	-1.1010421542
H	-3.9091118165	-0.5234708853	-2.1778403371
H	-4.934509545	-1.2963152049	-0.9632596637
H	-4.371441378	0.3645786918	-0.7166374189
H	-4.371441378	0.3645786918	-0.7166374189

TS 6-311++G(d,p) 0047

E(UwB97XD) = -1036.89276447 A.U.

First frequency = -1529.8511 cm⁻¹

S	-0.2097013971	1.4305535102	0.6906806567
O	0.7388697785	1.8667417191	1.709885644
O	-1.3983880993	2.2432899703	0.4506422542
N	-0.7415316407	-0.0708941795	1.1255876533
C	-1.9901641646	-0.5993222629	0.5627532018
H	-2.2371153505	-1.454166892	1.1972488306
H	-2.773300287	0.1440352708	0.7222439274
C	-1.9766143257	-1.0378009055	-0.92462232
H	-0.9336842377	-1.1076933927	-1.2475524433
C	0.2316339546	-1.0247319847	1.6725642955
H	-0.3242852284	-1.6710072549	2.3563046234
H	0.9400365991	-0.4628336789	2.2818093114
C	0.9674233906	-1.888342264	0.6422874994
H	0.2377992613	-2.4466939264	0.049230033
H	1.5423298391	-2.6398150263	1.2014062794
C	1.9195237483	-1.1323452302	-0.2726419755
H	1.3066331747	-0.0274364992	-0.575443141
C	3.1826909485	-0.6456952736	0.4083962661
H	3.7820707953	-0.031029932	-0.2682343584
H	3.7984912453	-1.4994142796	0.7184265834
H	2.9623850363	-0.0492505464	1.2975272672
C	2.1568793291	-1.8057664527	-1.6065839438
H	2.6737866118	-2.7636689485	-1.4646062358
H	2.7788595394	-1.1864607262	-2.2585265415

H	1.2145388853	-2.0118546287	-2.1227788947
C	0.6951554551	1.2100620495	-0.8135183419
H	-0.0036907737	0.9997456413	-1.6212136781
C	1.7690506881	2.2203783826	-1.1097204694
H	2.3304952659	1.8976261836	-1.9895780479
H	2.4603688872	2.314909726	-0.2710622903
H	1.349079153	3.2086699228	-1.3240640146
C	-2.6868741196	-0.0185492802	-1.8188813464
H	-2.2785061409	0.9871949611	-1.6957553723
H	-2.6049549901	-0.3002292614	-2.8722407783
H	-3.7513351675	0.0293485551	-1.5652610944
C	-2.6065661548	-2.4222174827	-1.0817818117
H	-3.6422344329	-2.4175932157	-0.7252450658
H	-2.6159580765	-2.7314617267	-2.1303173463
H	-2.058269868	-3.1765010859	-0.5092657067
H	-2.058269868	-3.1765010859	-0.5092657067

TS 6-311++G(d,p) 0048

E(UwB97XD) = -1036.89312402 A.U.

First frequency = -1490.8427 cm^{-1}

S	-0.1991075215	1.1805719472	0.3638173661
O	-0.2133133046	1.0862003551	1.8223148691
O	-1.1331602645	2.1082400137	-0.2704358089
N	-0.4524721533	-0.3153555994	-0.2963812594
C	-1.5311255468	-0.5250851868	-1.2659578722
H	-1.7723519945	0.438103054	-1.7170885163
H	-1.1275019803	-1.1671236949	-2.0577722152
C	-2.8065845763	-1.1605189137	-0.6973393153
H	-2.550606863	-2.1553762055	-0.3130522796
C	0.0119500353	-1.5135180348	0.4207519922
H	-0.0609170807	-2.3213632397	-0.312290122
H	-0.6710520005	-1.7603747535	1.2409600066
C	1.4412184049	-1.4587644556	0.9649279676
H	1.7114549686	-2.4871027755	1.2400751561
H	1.4621472291	-0.8783173058	1.8912644406
C	2.4823358891	-0.8989490248	0.0133789657
H	2.071610637	0.3122332827	-0.1190870158

C	3.8559206545	-0.7779213973	0.6364751058
H	4.5428796407	-0.2382480562	-0.0209127439
H	4.2826084493	-1.7728135199	0.8189195487
H	3.813443106	-0.2542742683	1.5956263935
C	2.477227385	-1.4828884535	-1.3822586392
H	1.5039777024	-1.3671370929	-1.8656649772
H	2.7124932537	-2.5547819232	-1.3491655469
H	3.2275804978	-0.9970635102	-2.0112875861
C	1.4476636435	1.5674863444	-0.1506504125
H	1.4249010167	1.7889839058	-1.2167785091
C	2.219972276	2.5118053682	0.7270688949
H	2.2490208078	2.1525633521	1.7573662166
H	1.7884841517	3.5185122012	0.7267804437
H	3.244798905	2.5873025139	0.3567183811
C	-3.8135941909	-1.343665451	-1.8329771838
H	-3.394787116	-1.941725169	-2.6478178855
H	-4.7153671935	-1.8470059399	-1.475214425
H	-4.1122035292	-0.3734876083	-2.2447769283
C	-3.4000057832	-0.3419641559	0.4465272061
H	-3.6723915173	0.6611489749	0.1042535517
H	-4.2994921412	-0.8258660623	0.8367528534
H	-2.6937081325	-0.2311774369	1.2739089598
H	-2.6937081325	-0.2311774369	1.2739089598

TS 6-311++G(d,p) 0056

E(UwB97XD) = -1036.89381439 A.U.

First frequency = -1493.8893 cm^{-1}

S	-0.1849673061	1.3583947482	0.6045895483
O	0.4181816106	1.6208813225	1.9106389398
O	-1.3103692838	2.1992054228	0.200216031
N	-0.6809824499	-0.2246460785	0.5007308539
C	-2.112665595	-0.5172904395	0.3524652893
H	-2.4640003141	-1.011182271	1.2664976433
H	-2.6589185352	0.4222022907	0.2616059241
C	-2.4072304848	-1.3896184044	-0.8710823152
H	-1.7915466757	-2.2958243326	-0.8058607126
C	0.0640194795	-1.2437379699	1.2638167409

H	-0.2923930782	-2.200742602	0.8764220801
H	-0.2188352522	-1.1977209876	2.3223940522
C	1.5888673794	-1.1961546535	1.1502895159
H	1.9643613414	-2.1430351133	1.5605801969
H	1.9812505838	-0.405071819	1.7947655219
C	2.1372655615	-0.9998653649	-0.2512302035
H	1.6685208366	0.1628137081	-0.5356074503
C	3.6401284287	-0.8249184794	-0.2843074171
H	3.9840490562	-0.5467330627	-1.2841641609
H	4.140039503	-1.7627121999	-0.0093754378
H	3.9681682275	-0.0553876245	0.4200124127
C	1.5988963997	-1.9417963226	-1.3048444434
H	1.981369799	-1.6812287776	-2.2951635749
H	0.5082113772	-1.9239547067	-1.3470678772
H	1.9110532789	-2.9717057208	-1.087209376
C	1.0826155821	1.4365354339	-0.6244510152
H	0.6063076216	1.4120304195	-1.6032621174
C	2.1515835551	2.4717359024	-0.4141485176
H	2.6163410694	2.361567497	0.5672538798
H	1.7575714183	3.4903705042	-0.4950894556
H	2.9219102133	2.3496222205	-1.1788166865
C	-2.0589231868	-0.6592423845	-2.1659061949
H	-2.2312691595	-1.3009146765	-3.0342201795
H	-2.6764912745	0.2382498294	-2.2787800336
H	-1.0106603077	-0.351291684	-2.1774318051
C	-3.8750607651	-1.8149743047	-0.8488076982
H	-4.1082130986	-2.4518258991	-1.7059237295
H	-4.1165898676	-2.3712185306	0.0615149065
H	-4.5319342045	-0.9394694883	-0.8940068067
H	-4.5319342045	-0.9394694883	-0.8940068067

TS 6-311++G(d,p) 0057

E(UwB97XD) = -1036.89336453 A.U.

First frequency = -1428.5335 cm⁻¹

S	0.0138091917	1.4639850823	-0.5865805609
O	-1.0533579894	2.3429655617	-0.1133677211
O	0.5758496338	1.7298734185	-1.9108536967

N	-0.564797931	-0.1056334283	-0.4987062651
C	-2.0266833432	-0.2830819179	-0.5005464111
H	-2.4935884365	0.6710870062	-0.2550807453
H	-2.3518268697	-0.5574586593	-1.5127196001
C	-2.5034615301	-1.3363477539	0.5044654698
H	-1.9654695013	-2.27385106	0.318732576
C	0.1235100562	-1.1207810235	-1.3244795321
H	-0.170340216	-1.0030973318	-2.3747768462
H	-0.2781108794	-2.0768576848	-0.9838248547
C	1.6504231471	-1.1654555006	-1.2385836932
H	2.0795975935	-0.3878894146	-1.8760580677
H	1.9601172135	-2.1250674989	-1.6731008433
C	2.2360699731	-1.0278802307	0.1542560517
H	1.8687504918	0.1632855948	0.4375787349
C	1.641950399	-1.9331497236	1.2097707037
H	1.886470539	-2.9806789057	0.9892472134
H	0.5548244328	-1.8453322963	1.2538053507
H	2.0447866856	-1.6999909813	2.19886455
C	3.7480828796	-0.9690303841	0.1647127065
H	4.1219399175	-0.2175344751	-0.5362333883
H	4.169836423	-1.9388356553	-0.1284761357
H	4.1269959706	-0.7301520908	1.1620843577
C	1.3451541985	1.4628481133	0.5738013726
H	2.1278566137	2.1209512085	0.2017804357
C	0.9673596056	1.5954106063	2.021928737
H	1.8603964246	1.4665860078	2.6376168255
H	0.240066196	0.8355531373	2.3126063724
H	0.5406785736	2.5785956856	2.2395149431
C	-3.9925733868	-1.598932345	0.2769990443
H	-4.1867400613	-1.9479951955	-0.7411642749
H	-4.3626314316	-2.3577129126	0.9711088557
H	-4.575334281	-0.6853902235	0.4379630884
C	-2.2338662575	-0.9023864123	1.9425855579
H	-2.5776369257	-1.6625367394	2.6492550822
H	-1.1682361379	-0.7415770709	2.1139572307
H	-2.7573632264	0.0330323137	2.1680296982
H	-2.7573632264	0.0330323137	2.1680296982

TS 6-311++G(d,p) 0058

E(UwB97XD) = -1036.89208487 A.U.

First frequency = -1507.1248 cm⁻¹

S	0.0029867858	1.0864563958	-0.9880058366
O	-1.0230915614	2.0869278585	-0.7068717567
O	0.3205599784	0.7774110024	-2.3788400715
N	-0.4602104194	-0.3069655081	-0.2441655626
C	-1.4936063853	-0.2653993854	0.7960478077
H	-1.2761994612	-1.0887841373	1.4861664895
H	-1.3829001264	0.6597915392	1.365369141
C	-2.9414277832	-0.3737277024	0.3065947729
H	-3.1328810302	0.4989128433	-0.3263200243
C	0.1006563454	-1.6012156127	-0.6683094451
H	-0.3911473481	-1.9529130728	-1.5793559007
H	-0.1686338	-2.2985476749	0.1271853454
C	1.6175520901	-1.6441421922	-0.8906950428
H	1.8550107246	-1.2288363603	-1.8732949031
H	1.8966307188	-2.706024138	-0.9297753402
C	2.465240768	-0.93952106	0.1516495414
H	2.1023364096	0.2884617354	-0.0047286423
C	2.1576383491	-1.2877148815	1.591451777
H	2.3783965116	-2.346539226	1.7807629439
H	1.1072921406	-1.1182635245	1.8396262766
H	2.7668587791	-0.6936633203	2.2775079849
C	3.9412027035	-0.9348454324	-0.1828141576
H	4.1170681566	-0.5731371808	-1.1996192155
H	4.3526760297	-1.9499774023	-0.1131898732
H	4.5013127627	-0.3015095598	0.5105064843
C	1.513262638	1.5475339139	-0.1907940219
H	2.1481041623	2.079700565	-0.8965665232
C	1.3806192872	2.1309722516	1.1894306198
H	2.3761930644	2.2827122999	1.6122142363
H	0.834083172	1.458842097	1.8556109398
H	0.8641918238	3.0950076047	1.17472196
C	-3.875279541	-0.3114846966	1.5156921378
H	-3.7132803387	-1.1701057674	2.177288579
H	-3.7147730487	0.5995150888	2.0997445069

H	-4.9211392281	-0.3279969666	1.1988898526
C	-3.1898431145	-1.6356148778	-0.5170326772
H	-2.931804431	-2.5346967094	0.0544169377
H	-4.2444963119	-1.7081943829	-0.79623656
H	-2.6036761717	-1.636268378	-1.4384795003
H	-2.6036761717	-1.636268378	-1.4384795003

TS 6-311++G(d,p) 0059

E(UwB97XD) = -1036.89144051 A.U.

First frequency = -1525.3057 cm^{-1}

S	-0.1664954922	1.0589962908	0.9280036341
O	0.1737403902	0.7844298176	2.3202822679
O	-1.2388243106	2.0103399347	0.6471014957
N	-0.5740371649	-0.3653369896	0.2181348431
C	-1.4757899788	-0.3522180236	-0.9386947494
H	-1.3243226847	0.5722443272	-1.5021505172
H	-1.1679940841	-1.1734511996	-1.5951786661
C	-2.9615213188	-0.4993094722	-0.5988963858
H	-3.235450966	0.3617361746	0.019404967
C	0.0578121214	-1.6238099904	0.6513652747
H	-0.1816256785	-2.3446931423	-0.1321647367
H	-0.4145763125	-1.9846873699	1.569050351
C	1.576343688	-1.5848218137	0.8676468066
H	1.9091881834	-2.6295760202	0.9379045055
H	1.7928767763	-1.1280999037	1.8367271528
C	2.3868526099	-0.8697775907	-0.1976006896
H	1.9363155734	0.3387809135	-0.1150471698
C	3.8541192807	-0.7498045582	0.1544507955
H	4.333695457	-1.7371832617	0.1393064663
H	3.9904953937	-0.3299679584	1.1549515055
H	4.3821765284	-0.1139815368	-0.5612468463
C	2.1257399468	-1.3015540958	-1.623862377
H	2.4014270415	-2.3554679461	-1.7597944363
H	2.7180814942	-0.7094733354	-2.3262405004
H	1.0741039567	-1.1952903813	-1.899329622
C	1.304516067	1.5731534788	0.0882612279
H	1.0354602039	1.8788340757	-0.9223493829

C	2.2313846299	2.4832791892	0.8451466661
H	3.141950311	2.6351843755	0.2613814095
H	2.5050420729	2.0485069348	1.8081182316
H	1.781829708	3.4654217194	1.026753845
C	-3.2442024173	-1.7762934791	0.1895168794
H	-2.7176259682	-1.7804927737	1.1466829299
H	-4.3133891998	-1.8710081351	0.3973458183
H	-2.9327355952	-2.6620852081	-0.3762835942
C	-3.7767345364	-0.4525744916	-1.8910333361
H	-4.8469624995	-0.5085543192	-1.6765712922
H	-3.5928522553	0.4712822737	-2.4473971878
H	-3.5225533997	-1.2961361978	-2.5429068546
H	-3.5225533997	-1.2961361978	-2.5429068546

TS 6-311++G(d,p) 0065

E(UwB97XD) = -1036.89277018 A.U.

First frequency = -1429.4573 cm⁻¹

S	-0.0526926785	1.3859130213	-0.3519770145
O	-1.1491562939	2.1728244383	0.2092609829
O	0.5298366022	1.8486687488	-1.6112694387
N	-0.6073369643	-0.1818389741	-0.4793007456
C	-2.0737615199	-0.3548522001	-0.4335964559
H	-2.5755788778	0.5004774046	-0.8924356407
H	-2.3016384497	-1.2235619065	-1.0586278162
C	-2.6219807536	-0.5883961694	0.9742481192
H	-2.2979805776	0.2522670926	1.5964467629
C	0.0796796334	-1.1188065352	-1.3966251798
H	-0.3250856691	-1.0044304872	-2.4094770431
H	-0.2058427427	-2.112849406	-1.0428056067
C	1.6050917198	-1.0350863057	-1.4811947091
H	1.8930242933	-0.1657629522	-2.076019115
H	1.9240350364	-1.9188365718	-2.0504761979
C	2.3588530536	-0.9972419611	-0.1640883622
H	1.9110869924	0.0829471175	0.359199228
C	2.029112374	-2.1047665425	0.8108852491
H	2.3584357008	-3.0723269935	0.4098675288
H	0.9566502555	-2.172495272	1.0011319395

H	2.5354733536	-1.951300683	1.7673186629
C	3.8413346205	-0.7452358082	-0.3351673016
H	4.0256691596	0.1388617887	-0.9515844507
H	4.3199423763	-1.601847273	-0.8268242987
H	4.331354877	-0.6008950003	0.6314602747
C	1.2499895864	1.2344223119	0.8249812178
H	1.9552547217	2.0503877326	0.6786546847
C	0.8259815634	0.9279976025	2.2336115113
H	1.7103104234	0.7213255193	2.8403975665
H	0.1777805616	0.0491331449	2.2634755594
H	0.2902535634	1.7675602866	2.6863568652
C	-2.0840521686	-1.8836692789	1.5760397141
H	-0.9924689912	-1.8812454717	1.6081504213
H	-2.4487293151	-2.0217734217	2.5974531964
H	-2.4033805829	-2.7488017191	0.9838662008
C	-4.149602174	-0.5927246721	0.9287604462
H	-4.5395705615	0.3534205981	0.542843948
H	-4.517576424	-1.3986759513	0.2837703957
H	-4.5673334805	-0.748613431	1.9267483861
H	-4.5673334805	-0.748613431	1.9267483861

TS 6-311++G(d,p) 0068

E(UwB97XD) = -1036.88720296 A.U.

First frequency = -1419.4411 cm⁻¹

S	-0.0960779786	1.1750632632	0.2592094092
O	0.3338318208	1.1199504608	1.6607568072
O	-1.0961323245	2.2007717325	-0.0405578086
N	-0.7234492627	-0.278454476	-0.2602443961
C	-1.9491909987	-0.6677221131	0.4586339962
H	-1.7018105513	-1.4153734223	1.222478557
H	-2.3442107423	0.2069653423	0.982759166
C	-3.034396887	-1.1985558755	-0.4818078566
H	-2.6155312976	-2.0346405536	-1.0549727752
C	0.1749492148	-1.3952389928	-0.6137312469
H	0.5854891108	-1.2134340173	-1.610640348
H	-0.4827446457	-2.2585322348	-0.7128763951
C	1.3059721637	-1.7162231971	0.375161205

H	1.5553021755	-2.7797054074	0.2762764081
H	0.9436847896	-1.5661481705	1.3958300546
C	2.5648494141	-0.8914808029	0.1269269156
H	2.0764013814	0.2089186847	-0.3043795692
C	3.3511892434	-0.5399576563	1.3685987473
H	4.1975190055	0.1105516199	1.1310942726
H	3.7520224105	-1.4499325366	1.8342996745
H	2.7152511901	-0.0363313476	2.1001346242
C	3.4094370617	-1.3869521087	-1.0290374729
H	3.8881100394	-2.3381565355	-0.7641229042
H	4.199416942	-0.6724383811	-1.2750790868
H	2.8126507737	-1.556933559	-1.9296766209
C	1.3420300931	1.3389013743	-0.7392027225
H	1.0967214994	1.1798656927	-1.7875079906
C	2.1886838314	2.5392687522	-0.4113812994
H	3.1114309588	2.4903018435	-0.9927690253
H	2.449248335	2.557196292	0.6486004802
H	1.6819380636	3.4765876837	-0.6620523179
C	-3.4918666784	-0.1233459504	-1.4638931837
H	-2.6483517788	0.2751901718	-2.0314961825
H	-4.2231938373	-0.5287470813	-2.1684222431
H	-3.9612520364	0.7095149731	-0.9295946574
C	-4.2015433066	-1.7344100725	0.347236544
H	-3.8807400931	-2.5323165253	1.0232112375
H	-4.6452240787	-0.9363138675	0.9523395869
H	-4.9844710854	-2.135376395	-0.3014332077
H	-4.9844710854	-2.135376395	-0.3014332077

TS 6-311++G(d,p) 0069

E(UwB97XD) = -1036.89099421 A.U.

First frequency = -1475.8256 cm⁻¹

S	-0.129508466	1.3125582217	0.2263034823
O	0.4010321844	1.8135129277	1.4943455346
O	-1.1732004636	2.1095735519	-0.416278922
N	-0.7257333834	-0.2343041566	0.389034025
C	-2.1881203635	-0.3913837582	0.2568135377
H	-2.4433307795	-1.2909107405	0.824547293

H	-2.7146047507	0.4397280731	0.7350645607
C	-2.675431692	-0.5606674311	-1.1835522275
H	-2.4401685972	0.3601437855	-1.7253568406
C	-0.109845838	-1.1224882853	1.3999879303
H	-0.4370564716	-2.127158386	1.1226248304
H	-0.526268008	-0.9046233105	2.3909005515
C	1.4169467654	-1.1048717293	1.4994798758
H	1.6912679642	-1.9557567748	2.1377421072
H	1.7420427432	-0.2064873144	2.0288163989
C	2.1727979989	-1.2011707908	0.1867249702
H	1.7596680026	-0.145907275	-0.4206417689
C	3.663513601	-0.9899292336	0.3416819796
H	4.159828585	-0.9431421456	-0.631383228
H	4.1102256245	-1.820608529	0.9033273998
H	3.8815959809	-0.0665595382	0.885317185
C	1.8043865642	-2.3725991863	-0.6954644535
H	0.7280975227	-2.4330873131	-0.8650510313
H	2.122983348	-3.3124749251	-0.2256840902
H	2.2997620978	-2.3035294626	-1.6675312014
C	1.2155089571	1.0623521244	-0.8880753594
H	0.8046182229	0.7811339207	-1.8566114086
C	2.2911133172	2.1118687395	-0.8767242458
H	1.9279175672	3.0745131566	-1.2520616559
H	3.1119802914	1.7902583783	-1.5213517744
H	2.6809102549	2.2619438791	0.1317499291
C	-4.1936899276	-0.7387964592	-1.1750361107
H	-4.6927680642	0.1051519563	-0.6898973353
H	-4.5803442951	-0.8175122621	-2.1943351947
H	-4.4762026863	-1.6521100023	-0.639119624
C	-1.9815560169	-1.7269092719	-1.8819003998
H	-0.9047320858	-1.5590084711	-1.9468374928
H	-2.149803193	-2.6648618799	-1.3396320943
H	-2.3654386361	-1.8533616715	-2.897901639
H	-2.3654386361	-1.8533616715	-2.897901639

TS 6-311++G(d,p) 0081

E(UwB97XD) = -1036.88964244 A.U.

First frequency = -1440.1376 cm⁻¹

S	0.0666206829	1.0037076707	-0.8489284185
O	-0.9508459619	2.0517052469	-0.8028996761
O	0.5660905323	0.6070343892	-2.1615538582
N	-0.5906747963	-0.306452831	-0.0892225642
C	-1.8383732898	-0.1266587488	0.6690067633
H	-1.788511622	-0.8125267894	1.5221874513
H	-1.8846133854	0.8856462775	1.075158866
C	-3.1028039427	-0.4072265507	-0.1466091092
H	-3.1237669356	0.3194759691	-0.9661019547
C	0.195882002	-1.5010664192	0.2857539181
H	-0.4783722933	-2.3500732271	0.15635991
H	0.4280569245	-1.4418023748	1.3571062682
C	1.4743227042	-1.7825783332	-0.5020575727
H	1.2718495657	-1.6929680692	-1.5706422409
H	1.7257689655	-2.8342737721	-0.3130198888
C	2.6829567461	-0.9332978417	-0.1239650821
H	2.2012915448	0.2496608018	-0.0026608022
C	3.2701784263	-1.2371306756	1.2390381108
H	4.0433047252	-0.5106625646	1.502916796
H	3.7334237079	-2.2321842621	1.2366978908
H	2.5146370253	-1.2257627489	2.0288825979
C	3.7099669232	-0.8197923985	-1.2279978191
H	4.5277437027	-0.1525869344	-0.9424548957
H	3.2524267735	-0.4404870971	-2.1450428462
H	4.1439185007	-1.8039694055	-1.4477281333
C	1.4756072475	1.4502354161	0.1103701776
H	2.072628171	2.1691479539	-0.4480352699
C	1.2293262819	1.7382171161	1.5647051308
H	2.184979422	1.8747965941	2.0749317402
H	0.7016867217	0.9147563433	2.0529870001
H	0.6394336114	2.6501690409	1.702299768
C	-4.3311275909	-0.1808056546	0.7338830982
H	-4.3410982676	-0.8824412581	1.5757178901
H	-4.3501082223	0.8346333993	1.1404319419
H	-5.2510125998	-0.3324516821	0.1633619887
C	-3.0980605449	-1.8118837199	-0.7454030634
H	-4.000622079	-1.9816451669	-1.3386477918
H	-2.2346524084	-1.9608659041	-1.3990046223

H	-3.0685099191	-2.571934758	0.0441221293
H	-3.0685099191	-2.571934758	0.0441221293

TS 6-311++G(d,p) 0082

E(UwB97XD) = -1036.88715891 A.U.

First frequency = -1427.9342 cm⁻¹

S	-0.156538293	1.1064780527	0.1836196485
O	0.1681024311	1.0138893562	1.6044116894
O	-1.1163260121	2.1368657987	-0.2073394573
N	-0.7643942245	-0.3516788799	-0.3257199301
C	-1.9271901608	-0.3566738589	-1.2310968915
H	-2.0640722902	0.6417940119	-1.6468666186
H	-1.6896547029	-1.0268999999	-2.0642797183
C	-3.2324293541	-0.8016634173	-0.5573055457
H	-3.9816414189	-0.7933719323	-1.359528533
C	0.1264792736	-1.5230004042	-0.4818244495
H	0.5691325314	-1.5063410187	-1.4876288276
H	-0.533836606	-2.3883606747	-0.4446532449
C	1.2240099693	-1.7039959725	0.5689410123
H	1.4735874349	-2.7720344329	0.5895158921
H	0.8269003618	-1.4509094749	1.5537519188
C	2.5025489183	-0.9195233737	0.2906143612
H	2.0537694769	0.1704566467	-0.2086715024
C	3.2679808263	-0.5178274324	1.530454948
H	4.1354913919	0.09869595	1.2790865961
H	3.6351536144	-1.409199039	2.0562140627
H	2.6274545441	0.0398628871	2.2176663452
C	3.3643357043	-1.5004059427	-0.8114280328
H	4.1790834449	-0.8201994733	-1.0736499021
H	2.7893914082	-1.7055929835	-1.7186623131
H	3.8114978739	-2.446471177	-0.4805607406
C	1.3659005805	1.3039610787	-0.6842793164
H	1.2061455428	1.1373311398	-1.7489512904
C	2.1897674052	2.5008225529	-0.2947337732
H	1.700271647	3.4394396024	-0.5739353853
H	3.1516515025	2.457421521	-0.8101521784
H	2.3758992192	2.5138026777	0.7809691592

C	-3.6791031062	0.1826042513	0.5222664194
H	-3.7744615612	1.1954219344	0.1243585682
H	-4.6433172626	-0.1190237855	0.9408383867
H	-2.9522117354	0.2127628534	1.3401462545
C	-3.1552382208	-2.2221998436	0.0017564294
H	-4.1282421107	-2.5330911627	0.3915701603
H	-2.8555002898	-2.94352823	-0.7648162431
H	-2.4378724414	-2.2756029188	0.8270001414
H	-2.4378724414	-2.2756029188	0.8270001414

TS 6-311++G(d,p) 0089

E(UwB97XD) = -1036.88519226 A.U.

First frequency = -1419.4291 cm⁻¹

S	-0.1588203394	1.0915536335	0.4591787125
O	0.4176617267	0.9404425557	1.8000188303
O	-1.2052211284	2.1077257368	0.349746023
N	-0.8006898039	-0.3380293127	-0.1093181988
C	-1.9766717714	-0.7934424263	0.661239861
H	-1.7146290913	-1.7243715765	1.1760148899
H	-2.197981172	-0.0599906725	1.44045351
C	-3.2390383836	-0.9875600273	-0.1890252975
H	-3.999299225	-1.3412877397	0.5192429873
C	0.1014363339	-1.4011356059	-0.6032207394
H	0.403976971	-1.1541778273	-1.6249696212
H	-0.5279334405	-2.2848642741	-0.6812809946
C	1.3360486538	-1.7282754845	0.2509163531
H	1.6068570143	-2.7747251738	0.0645045293
H	1.0727356575	-1.6493196377	1.308843181
C	2.5393382629	-0.847554326	-0.0696178054
H	1.9779793952	0.2566054753	-0.3828006607
C	3.4345567914	-0.5403429294	1.108482591
H	3.9032628681	-1.4613294493	1.47961901
H	2.8595766033	-0.0987409412	1.9255239065
H	4.2358374092	0.1492363699	0.8286278436
C	3.2789079462	-1.2480504996	-1.3297032831
H	4.0189440176	-0.4936855427	-1.6097654916
H	2.6006699852	-1.3891838584	-2.1760378736

H	3.809694977	-2.1949576037	-1.1688673188
C	1.1629424009	1.3790103277	-0.664898475
H	0.8177008148	1.2753607151	-1.6917105431
C	1.9957033574	2.590811781	-0.3435577604
H	2.3618432244	2.5540638231	0.6843081899
H	1.4334755502	3.5199805858	-0.4804034823
H	2.8562365602	2.6168148741	-1.0149503686
C	-3.081782108	-2.0544635979	-1.2727187203
H	-4.0372944735	-2.2253784046	-1.7756806952
H	-2.3618840921	-1.7388147627	-2.0343754051
H	-2.7481615726	-3.0103105946	-0.8570229369
C	-3.7225292577	0.3304681518	-0.7899858458
H	-4.6544535275	0.1802552343	-1.3421692386
H	-3.8957763478	1.0817534521	-0.0159837709
H	-2.9755192282	0.7333007974	-1.4793700828
H	-2.9755192282	0.7333007974	-1.4793700828

7 Enantioselective dialkylzinc additions on benzaldehyde

7.1 25 *anti pro-R*

7.1.1 Starting TS

TS input

E(RB-P86) = -5316.45242351 A.U.

First frequency = -196.2901 cm⁻¹

C	2.67809	-1.78196	-0.16461
C	4.06831	-0.53681	-1.6983
C	4.69331	-1.7133	-2.13779
C	4.32835	-2.94609	-1.58292
C	3.32791	-2.96365	-0.60385
C	1.62935	-2.08254	0.87682
C	2.01107	-2.50348	2.16617
C	1.0348	-3.02825	3.02751
C	-0.2825	-3.15062	2.57484

C	-0.61298	-2.70474	1.27285
H	4.40061	0.40495	-2.14736
H	5.47085	-1.65617	-2.91614
H	4.80555	-3.8833	-1.90884
H	3.0188	-3.92472	-0.16237
H	3.0656	-2.43879	2.47103
H	1.30902	-3.36774	4.0389
H	-1.05369	-3.61342	3.20646
N	0.33768	-2.1654	0.46658
C	2.44259	0.8198	-0.18432
C	2.61234	2.07615	-1.17019
C	3.31449	1.34588	1.11896
C	4.04554	2.58414	-0.84723
C	1.77767	3.24945	-0.55676
C	3.7932	2.76997	0.66331
H	4.27125	3.54326	-1.36225
H	4.86978	1.88221	-1.07233
H	1.63046	4.03193	-1.33025
H	0.77038	2.90039	-0.26014
C	2.62888	3.77663	0.63293
H	4.66528	3.11651	1.25691
H	3.01862	4.79669	0.43172
H	2.0734	3.83497	1.58897
C	4.5745	0.49964	1.41735
H	4.32131	-0.5457	1.68366
H	5.2813	0.45439	0.56585
H	5.11721	0.94176	2.28028
C	2.47615	1.36717	2.40207
H	2.16696	0.34419	2.69614
H	3.06807	1.79799	3.23845
H	1.55252	1.97095	2.31561
C	2.20071	1.86063	-2.62871
H	1.12178	1.60519	-2.68492
H	2.35133	2.79468	-3.21098
H	2.74586	1.04918	-3.14651
C	3.05306	-0.51204	-0.71012
O	1.07596	0.55683	0.07471
C	-1.98782	-2.87051	0.73036

C	-2.18575	-3.14032	-0.64392
C	-3.11789	-2.80685	1.57958
C	-3.47704	-3.34246	-1.15322
H	-1.31457	-3.20597	-1.31288
C	-4.40943	-3.004	1.06696
H	-2.98917	-2.56829	2.64656
C	-4.59332	-3.27551	-0.30091
H	-3.61118	-3.55706	-2.22499
H	-5.27883	-2.9386	1.74021
H	-5.6068	-3.43362	-0.70254
Zn	0.0655	-0.7573	-1.17185
C	-0.04243	-1.24504	-3.10164
H	-1.12629	-1.36355	-3.33375
H	0.29057	-0.37769	-3.71421
C	-1.79181	3.03879	0.85038
C	-1.88448	1.38808	-0.75915
H	-1.12954	1.90306	-1.39692
Zn	-0.51913	1.11718	1.2635
O	-1.60747	0.17552	-0.31764
H	-2.77007	2.73607	1.27533
H	-1.99304	3.66409	-0.0391
C	-0.91797	0.58684	3.15392
H	-0.2811	1.20159	3.82865
H	-0.55238	-0.45755	3.2689
C	-3.29403	1.70486	-1.09397
C	-3.61248	2.80801	-1.9202
C	-4.34003	0.88108	-0.6167
C	-4.94614	3.08927	-2.25376
H	-2.80148	3.44265	-2.31527
C	-5.67238	1.16464	-0.94999
H	-4.07933	0.0102	0.00375
C	-5.98101	2.27019	-1.76564
H	-5.18075	3.94832	-2.90246
H	-6.48022	0.51593	-0.57481
H	-7.02866	2.49028	-2.02651
C	-0.99494	3.88562	1.8614
H	-0.00558	4.2034	1.47399
H	-1.55324	4.82566	2.08878

H	-0.82704	3.37111	2.83025
C	-2.38873	0.6865	3.57912
H	-2.55749	0.34218	4.62732
H	-2.76924	1.72975	3.52889
H	-3.05413	0.07883	2.92877
C	0.72973	-2.50264	-3.53141
H	0.59295	-2.74871	-4.61113
H	1.82279	-2.39573	-3.36302
H	0.4173	-3.40815	-2.96333
H	0.4173	-3.40815	-2.96333

7.1.2 Lowest TS

TS 0001

E(RB-P86) = -5316.45897960 A.U.

First frequency = -195.3715 cm⁻¹

C	-2.8327465556	1.589204044	-0.0177074342
C	-4.1803275328	0.3768567214	-1.6149795856
C	-4.9065170224	1.5342418102	-1.9314427012
C	-4.6096537335	2.7413116433	-1.2863281482
C	-3.582540569	2.7510590716	-0.335541271
C	-1.7973763958	1.8736192671	1.0412246471
C	-2.2051343613	2.1542609219	2.3609606159
C	-1.2674399934	2.6677095612	3.2703067401
C	0.039872633	2.9124345896	2.8385908644
C	0.3985475526	2.6017921913	1.5055448715
H	-4.4612868433	-0.5482833847	-2.1293915015
H	-5.7082406508	1.4828105356	-2.6852863631
H	-5.1636731765	3.6643137282	-1.5175340917
H	-3.333008833	3.6911653724	0.1821406223
H	-3.2527416571	1.9914496057	2.6529081468
H	-1.564543754	2.8998000219	4.3053045978
H	0.7818805512	3.3642183345	3.5119088212
N	-0.5144143454	2.0786743865	0.6471445286
C	-2.3903532418	-0.973538996	-0.3023573886
C	-2.4732472796	-2.1205231262	-1.4292403477
C	-3.1753940754	-1.7209347557	0.9431748864

C	-3.8257398876	-2.8231156397	-1.1235452027
C	-1.4949447829	-3.2558708373	-0.9894245274
C	-3.4921523682	-3.1382322703	0.3504058407
H	-3.9608698406	-3.7409850113	-1.7362675036
H	-4.7337483078	-2.2034975041	-1.2467285953
H	-1.3255532545	-3.9376850445	-1.8489797303
H	-0.5130837113	-2.8374497938	-0.7084428618
C	-2.213595391	-3.9841871346	0.1802291364
H	-4.2919962969	-3.6513239506	0.9249853946
H	-2.4849141072	-5.0250554879	-0.0946994055
H	-1.6025539176	-4.0542072721	1.102181764
C	-4.5167239752	-1.053720251	1.3295911324
H	-4.3727266844	-0.0196099499	1.7013948335
H	-5.2368330915	-0.9980368244	0.490326714
H	-4.9964060116	-1.6379311639	2.1439801663
C	-2.3263544595	-1.7703148829	2.2175669478
H	-2.1145834498	-0.7521515558	2.6007330053
H	-2.8643331923	-2.3304284674	3.0125107168
H	-1.3491647715	-2.2733134092	2.0788775901
C	-2.152764651	-1.69662895	-2.8650752214
H	-2.8085451955	-0.9032703907	-3.2700576617
H	-1.1132582293	-1.3114913787	-2.9249876189
H	-2.2218684338	-2.5718285809	-3.5458810357
C	-3.1259742498	0.347812397	-0.6683180763
O	-1.0465636013	-0.6259513256	-0.0251699423
C	1.7651671762	2.8878020376	0.9941482623
C	1.952219563	3.3399169247	-0.3326501431
C	2.8957746376	2.7493311181	1.833135026
C	3.236139162	3.649786811	-0.8055291017
H	1.078663144	3.4620495087	-0.9907259738
C	4.1798529241	3.0540529524	1.3557391293
H	2.7718241766	2.3638305834	2.8571193887
C	4.3538208552	3.5089195385	0.0359663084
H	3.3635565651	4.0070843744	-1.8394147823
H	5.0516405286	2.9289039266	2.0174286403
H	5.3613922342	3.7518164935	-0.3373050649
Zn	-0.1409211688	0.8701866201	-1.1191334417
C	-0.0608831539	1.5659500851	-2.9852065487

H	1.0049199153	1.8325617065	-3.173809828
H	-0.2791630041	0.7355663124	-3.693452548
C	1.6701588005	-3.0767424125	0.5648195286
C	1.945929633	-1.1789850513	-0.9233027007
H	1.2118159258	-1.6792503	-1.5956629431
Zn	0.5733015164	-1.2037964849	1.1312630109
O	1.6258014169	-0.0280507081	-0.388035001
H	1.7041428658	-3.6012065466	-0.409585005
H	0.7937508464	-3.5213550776	1.0999398277
C	1.0361705053	-0.6929041485	3.0169852666
H	0.4916729466	0.247100364	3.2529657256
H	2.1155769726	-0.4203317243	2.9861585842
C	3.3616269515	-1.4730930878	-1.2173261713
C	3.7128588998	-2.5414031679	-2.0770514936
C	4.3864468346	-0.6610178581	-0.674771604
C	5.0577872655	-2.8012649058	-2.3771960684
H	2.9187424	-3.1658041567	-2.5191914618
C	5.7303679227	-0.9220449586	-0.9792935594
H	4.098461032	0.180957433	-0.0269857478
C	6.0713119764	-1.9934489137	-1.8268414012
H	5.319858003	-3.6335509364	-3.0497695884
H	6.521967466	-0.2834141566	-0.5554395301
H	7.1279002458	-2.1962433621	-2.0644427818
C	2.9387290782	-3.2795262089	1.3810031112
H	2.8663919982	-2.8175247904	2.3865171845
H	3.1623619529	-4.3614185807	1.5350831729
H	3.8314545239	-2.8434777047	0.8852805976
C	0.7862827858	-1.7313850273	4.118986474
H	1.3134919989	-2.691468505	3.9263515428
H	1.1290426601	-1.3825224874	5.1220565927
H	-0.2912472154	-1.9806770556	4.2268391381
C	-0.9691127431	2.764378048	-3.3036228789
H	-0.8481921849	3.1360182627	-4.348747475
H	-2.044450636	2.5159072829	-3.1743637594
H	-0.7716039816	3.6346486927	-2.6375940563
H	-0.7716039816	3.6346486927	-2.6375940563

7.1.3 Additional TS

TS 0006

E(RB-P86) = -5316.45832710 A.U.

First frequency = -194.0450 cm⁻¹

C	-2.8214311262	1.6113218329	0.1602875444
C	-4.2703090101	0.5599501643	-1.461614431
C	-4.9531851206	1.7645451192	-1.6820241498
C	-4.5799117249	2.9163043062	-0.977506633
C	-3.5255560166	2.822966622	-0.0617854467
C	-1.741184116	1.7890976502	1.1990125326
C	-2.0870042092	1.9380347876	2.5564790071
C	-1.1114794766	2.3904002895	3.4587168871
C	0.1601928593	2.7243022718	2.9828117937
C	0.4581821817	2.5465767409	1.6107854444
H	-4.6058254562	-0.3186048766	-2.023276499
H	-5.7802304885	1.7947784526	-2.4092163427
H	-5.0983181642	3.8750130808	-1.1344630116
H	-3.2192795965	3.7169395253	0.505024503
H	-3.1151823829	1.7272249541	2.8843075594
H	-1.3556808659	2.5172541368	4.5252949694
H	0.915336981	3.1489266332	3.6585190014
N	-0.4834362586	2.0548705599	0.7620568033
C	-2.4762770746	-0.9320591821	-0.316338416
C	-2.6037249734	-1.9727400239	-1.5406651395
C	-3.253831464	-1.7719780149	0.8732266475
C	-3.958347936	-2.6837339362	-1.2661187719
C	-1.6328268025	-3.1539805836	-1.2297050933
C	-3.5972208019	-3.1289800047	0.1666902638
H	-4.1179972854	-3.5429664083	-1.953472387
H	-4.8612357653	-2.0465949293	-1.3148160996
H	-1.5025715652	-3.763670524	-2.1482356117
H	-0.6364333629	-2.7734493035	-0.9472226203
C	-2.330534199	-3.9675951647	-0.1037902089
H	-4.3896376664	-3.6838257211	0.7120631848
H	-2.6172798556	-4.9814795019	-0.4536381566
H	-1.6985768124	-4.1158891634	0.7948941362
C	-4.5804829341	-1.1195147145	1.3303713434

H	-4.4155022508	-0.1214409123	1.7836312676
H	-5.3095607861	-0.9836680224	0.5083334211
H	-5.0597023088	-1.7616149336	2.1001876337
C	-2.3969432209	-1.9441737663	2.1320913811
H	-2.173060938	-0.9673731869	2.6045913589
H	-2.9384160259	-2.5656831236	2.8776017996
H	-1.4271034728	-2.4449375691	1.9454108078
C	-2.3147322603	-1.4268561247	-2.9410287435
H	-2.9785339296	-0.6014008176	-3.2595463344
H	-1.2750171037	-1.0409490847	-2.9928800094
H	-2.4043785859	-2.2402087261	-3.6924667991
C	-3.1869065314	0.4296822979	-0.5571848115
O	-1.1204953972	-0.6331596801	-0.0364049264
C	1.7706230166	2.9633545371	1.0451108977
C	1.8661866484	3.3771999325	-0.3046073519
C	2.9357267984	3.0129395624	1.8480662278
C	3.0874661065	3.8179822362	-0.8354080354
H	0.9669052225	3.3628567728	-0.9376804727
C	4.1577238809	3.4508205708	1.3148391273
H	2.8969322391	2.6811147701	2.8966208624
C	4.2388958162	3.8554882229	-0.0295096303
H	3.1375237405	4.1389568299	-1.8876999398
H	5.0544913229	3.4707756453	1.9542233955
H	5.1979102876	4.2003516497	-0.4475888385
Zn	-0.1938107868	0.8970050782	-1.0659544512
C	-0.2421871582	1.6722817747	-2.9043345428
H	-1.2567272735	1.5028281327	-3.3287069027
H	-0.1568569964	2.780010019	-2.8114616487
C	1.4982925767	-3.1594078753	0.344605171
C	1.9296622057	-1.1457586454	-0.9175122007
H	1.2668474808	-1.5843378439	-1.697363615
Zn	0.4939695956	-1.2916184752	1.0799568768
O	1.5606962145	-0.0262504859	-0.3412650468
H	1.6126717417	-3.5578860114	-0.6812657344
H	0.542432205	-3.6024049684	0.7175142893
C	0.830580193	-1.0042420611	3.0359591911
H	0.5791327247	-1.963526503	3.5442961657
H	0.0721303824	-0.2709675567	3.3897074731

C	3.3687662652	-1.4335817787	-1.0825625588
C	3.8062903944	-2.4230070767	-1.9953900831
C	4.3329531167	-0.6950777107	-0.3558043568
C	5.1745401518	-2.676280932	-2.1701019511
H	3.0624941256	-2.9892754608	-2.580277551
C	5.7006958583	-0.9496155021	-0.5338990262
H	3.9823792978	0.08660735	0.3348855527
C	6.1264295809	-1.9416317266	-1.4376796581
H	5.5034432579	-3.4457379967	-2.8866756067
H	6.4441213979	-0.3677806095	0.0342554366
H	7.2014221061	-2.139488091	-1.576068502
C	2.6530979881	-3.55460236	1.2529344203
H	2.4399201078	-3.3225911854	2.3160805045
H	2.8688646516	-4.6471732414	1.1936429915
H	3.5986894326	-3.0357529044	0.9839536602
C	2.2356635941	-0.5454893883	3.4468199347
H	2.3366660682	-0.4000524165	4.5490717464
H	3.0194196591	-1.2749410709	3.1514637119
H	2.5139857157	0.4166498981	2.967479008
C	0.8306396369	1.151222472	-3.8751640271
H	0.7867123785	1.6406577514	-4.8767585386
H	1.8600489147	1.3107356939	-3.4865228807
H	0.732654532	0.0580284535	-4.0588067224
H	0.732654532	0.0580284535	-4.0588067224

TS 0013

E(RB-P86) = -5316.45195477 A.U.

First frequency = -197.8771 cm^{-1}

C	-2.8138997459	1.6098724533	0.0034575158
C	-4.1525523669	0.4381864119	-1.6301492249
C	-4.834439459	1.6172128907	-1.9649681813
C	-4.5187874102	2.8149712564	-1.311659688
C	-3.5185215721	2.7939812612	-0.3326120692
C	-1.788250874	1.8636682481	1.0799774277
C	-2.2010038013	2.1225442043	2.4020418247
C	-1.262467969	2.6130553913	3.3233963705
C	0.0460588041	2.8632028883	2.8992084284

C	0.4086240733	2.5787739135	1.5610913136
H	-4.4444566182	-0.4766000673	-2.1565286641
H	-5.6158590335	1.590244304	-2.7410871977
H	-5.0386835908	3.7540273199	-1.5572820248
H	-3.2549854532	3.7257934151	0.1932518783
H	-3.2509996267	1.9625079862	2.6867844266
H	-1.5608841274	2.8273432094	4.3618657467
H	0.7842007279	3.3035899687	3.5839689769
N	-0.5032908049	2.068801309	0.6930870538
C	-2.420215508	-0.9578253478	-0.2805044291
C	-2.5123571839	-2.1033999197	-1.4040435062
C	-3.2324391494	-1.6863570327	0.9586847278
C	-3.8947720493	-2.7575035448	-1.1264496407
C	-1.5786568548	-3.2670294506	-0.9368085576
C	-3.6014347821	-3.0861637816	0.3526087755
H	-4.0527077833	-3.6700208831	-1.7417060742
H	-4.7763559387	-2.1044561182	-1.266232325
H	-1.3945971101	-3.9488761494	-1.793324431
H	-0.5932961036	-2.8740935177	-0.6230326105
C	-2.3575610077	-3.9817219888	0.2037155022
H	-4.43170285	-3.5670461425	0.9116292143
H	-2.6645064575	-5.0059848876	-0.0956679377
H	-1.7776368835	-4.0874884154	1.140248396
C	-4.5507856769	-0.9767682863	1.3473792161
H	-4.3754692468	0.0522092981	1.7194287905
H	-5.2684912308	-0.8990258711	0.5075245325
H	-5.0483550192	-1.5461739515	2.1615924529
C	-2.3853598278	-1.7779010484	2.2340658579
H	-2.1762801323	-0.7717580804	2.6488401883
H	-2.9261540959	-2.3613660755	3.0102193324
H	-1.405626595	-2.2718053201	2.0814585237
C	-2.143433843	-1.6892119356	-2.8308191833
H	-2.7803436323	-0.8925673175	-3.2585131713
H	-1.0990026107	-1.3122587838	-2.8586732747
H	-2.1978653426	-2.5661462412	-3.5105743547
C	-3.1247070419	0.3784026102	-0.6568474496
O	-1.0715763759	-0.6310945538	-0.0013738505
C	1.7708731071	2.8931604061	1.0530076767

C	1.9555222476	3.3091382928	-0.2863517085
C	2.898382787	2.8316519413	1.9059184162
C	3.2300878355	3.6582272164	-0.756704639
H	1.0853754966	3.3700663552	-0.9572957927
C	4.1736892768	3.1764281845	1.4318890758
H	2.7823915378	2.4801344642	2.9428982289
C	4.3435266258	3.5949241678	0.0998109329
H	3.3534346283	3.9854948469	-1.8009341418
H	5.0418435783	3.1119585515	2.1068851113
H	5.3437716205	3.8692103446	-0.2712271741
Zn	-0.1766784266	0.8757127627	-1.1073166863
C	-0.2720048681	1.607759321	-2.9585683552
H	-1.2868919733	1.3979302886	-3.364474465
H	-0.2188515744	2.7192813012	-2.8878310385
C	2.0042540101	-2.9355587309	0.5616844754
C	1.9871203109	-1.1360428485	-0.9209815852
H	1.3133276437	-1.6735803887	-1.6267754372
Zn	0.5704279171	-1.1995317197	1.1107069699
O	1.5714572646	-0.006339173	-0.3883063443
H	2.8356841357	-2.5608755451	1.1957338026
H	2.4610938147	-3.3885290782	-0.3361533592
C	1.0190501918	-0.6745528356	2.9943403035
H	0.2119023894	0.0144949576	3.3266395499
H	1.9331622494	-0.0470143109	2.8898011413
C	3.435202095	-1.2791063023	-1.2076951293
C	3.8987783359	-2.2446410493	-2.132244441
C	4.3716223572	-0.4237311483	-0.5822210529
C	5.2671298541	-2.3589383145	-2.4200163972
H	3.173145115	-2.9029507033	-2.6390819283
C	5.7396986958	-0.5424424982	-0.8682734143
H	3.9994676146	0.3408187541	0.11647992
C	6.1928956182	-1.5102290059	-1.7847673314
H	5.61473741	-3.1101360886	-3.1471181096
H	6.4614861752	0.1289870729	-0.3759736398
H	7.26794113	-1.5999945008	-2.008938058
C	1.1914578649	-4.0315766055	1.2731289205
H	0.7006820747	-3.6951341824	2.210451121
H	0.4069810962	-4.462667781	0.619572457

H	1.860580677	-4.8795840439	1.5565768854
C	1.2525133881	-1.7599485668	4.0506754522
H	1.527506541	-1.3338608293	5.0446499062
H	0.3491989971	-2.3864573511	4.2200054236
H	2.074798882	-2.4527882281	3.7695256301
C	0.8034472593	1.0980536981	-3.9322014361
H	0.730597862	1.562149771	-4.9442418415
H	1.8324709938	1.2986583241	-3.562159898
H	0.7381595554	-0.0016325798	-4.088583003
H	0.7381595554	-0.0016325798	-4.088583003

7.2 26 *anti pro-S*

7.2.1 Starting TS

TS input

E(RB-P86) = -5316.44652052 A.U.

First frequency = -196.4149 cm⁻¹

C	2.36871	-1.87145	-0.66832
C	3.61798	-0.43929	-2.15919
C	4.1376	-1.54913	-2.84209
C	3.79392	-2.84347	-2.43286
C	2.91373	-2.98678	-1.3537
C	1.4296	-2.29862	0.43081
C	1.93062	-2.92643	1.58853
C	1.02999	-3.5354	2.47626
C	-0.33489	-3.53413	2.17228
C	-0.78288	-2.88559	0.99695
H	3.93361	0.55185	-2.50116
H	4.81795	-1.39172	-3.69416
H	4.19244	-3.73079	-2.94877
H	2.61712	-3.9962	-1.02637
H	3.01483	-2.95048	1.77053
H	1.39696	-4.03417	3.38725
H	-1.05684	-4.05505	2.81699
N	0.09804	-2.26728	0.16898
C	2.27341	0.70811	-0.25133

C	2.40056	2.10234	-1.03608
C	3.33605	0.97078	0.98965
C	3.89177	2.49018	-0.82763
C	1.72471	3.18961	-0.13855
C	3.8393	2.43162	0.71346
H	4.10929	3.51207	-1.20759
H	4.63841	1.80359	-1.26784
H	1.53129	4.09594	-0.74936
H	0.7428	2.83528	0.22022
C	2.74319	3.47412	0.99994
H	4.79779	2.63727	1.23486
H	3.16702	4.49721	0.91977
H	2.31104	3.39344	2.01666
C	4.57103	0.03877	0.97235
H	4.29259	-1.02627	1.09725
H	5.15987	0.11179	0.03732
H	5.24418	0.30892	1.81403
C	2.67432	0.80256	2.36041
H	2.33721	-0.24175	2.51638
H	3.39517	1.05426	3.16775
H	1.7886	1.45128	2.51004
C	1.7961	2.15161	-2.44168
H	0.70159	1.9776	-2.38601
H	1.94678	3.15775	-2.8877
H	2.20455	1.40386	-3.14708
C	2.73274	-0.54236	-1.05725
O	0.93363	0.46053	0.14749
C	-2.21841	-2.91169	0.61013
C	-3.23556	-2.87275	1.59231
C	-2.5894	-3.0154	-0.75056
C	-4.58784	-2.92982	1.22191
H	-2.9659	-2.75682	2.65368
C	-3.9418	-3.07914	-1.11791
H	-1.80556	-3.05846	-1.52187
C	-4.94571	-3.03573	-0.13418
H	-5.36857	-2.88248	1.99767
H	-4.21326	-3.16559	-2.18179
H	-6.00745	-3.0823	-0.42419

Zn	-0.30293	-0.56783	-1.16214
C	-0.59113	-0.8199	-3.12209
H	-1.69385	-0.87505	-3.27457
H	-0.26617	0.09308	-3.67013
C	-1.52934	2.94756	1.42862
C	-2.55586	1.07218	0.40509
H	-3.19599	0.9863	1.31241
Zn	-0.38205	0.90704	1.65792
O	-1.76951	0.06353	0.1672
H	-1.16424	3.44125	0.50427
H	-2.60953	3.17203	1.49823
C	-0.77915	0.07791	3.44855
H	-1.85201	0.32993	3.6177
H	-0.75497	-1.02275	3.28388
C	-3.14436	1.90325	-0.67203
C	-2.55476	2.00224	-1.95318
C	-4.34527	2.61083	-0.42172
C	-3.1487	2.78515	-2.95368
H	-1.62816	1.44721	-2.16294
C	-4.94031	3.39326	-1.42225
H	-4.82166	2.53074	0.56988
C	-4.3423	3.48428	-2.69278
H	-2.67747	2.84852	-3.94735
H	-5.87822	3.93201	-1.21288
H	-4.8078	4.09792	-3.48054
C	0.08612	-2.05221	-3.74295
H	1.193	-1.99615	-3.67287
H	-0.20784	-2.99897	-3.23604
H	-0.16275	-2.18383	-4.82238
C	0.03639	0.42934	4.69889
H	0.04575	1.52121	4.9073
H	-0.35973	-0.06253	5.61898
H	1.09869	0.11665	4.61037
C	-0.85704	3.50947	2.69387
H	-1.23079	3.01979	3.61705
H	0.24996	3.40811	2.69899
H	-1.06835	4.60126	2.80229
H	-1.06835	4.60126	2.80229

7.2.2 Lowest TS

TS 0001

E(RB-P86) = -5316.45414105 A.U.

First frequency = -194.2597 cm⁻¹

C	2.6155879893	-1.6406094672	-0.4032922771
C	3.8892633883	-0.1781162694	-1.8446579621
C	4.5747396383	-1.266797377	-2.4022171738
C	4.2956124129	-2.5658056154	-1.958884148
C	3.3257615417	-2.7339854123	-0.9640673578
C	1.6380128486	-2.1013278132	0.6485549751
C	2.1242653353	-2.6249537912	1.8639875567
C	1.2379565481	-3.2935642192	2.7220510174
C	-0.0984984561	-3.4444258625	2.3394961726
C	-0.5361490568	-2.884558766	1.1161547397
H	4.1558178198	0.8213611	-2.204747375
H	5.3313495902	-1.0899937427	-3.1832246323
H	4.8191114463	-3.4382326575	-2.3798401442
H	3.0897759282	-3.7484273929	-0.6046530005
H	3.1914250411	-2.5256657473	2.1103828987
H	1.5961863806	-3.7168015576	3.6738442627
H	-0.8046493603	-4.0098536991	2.9638053783
N	0.3285674334	-2.2166326163	0.309156604
C	2.2189663753	0.9400285059	-0.2058810649
C	2.2154828759	2.2505236782	-1.1463852487
C	3.1267101567	1.4829650462	1.0608864348
C	3.5841007895	2.9204105931	-0.8402183456
C	1.2697017761	3.2851913191	-0.4619343076
C	3.3724373732	2.9851788527	0.6865518419
H	3.6585677324	3.9278315311	-1.3045775485
H	4.4839840325	2.350112352	-1.1384051332
H	1.0477357815	4.1000575255	-1.1820681696
H	0.3053599534	2.8169296937	-0.1976997189
C	2.0718695545	3.8143471069	0.7607446659
H	4.2108484859	3.4195939669	1.2709787449
H	2.3079084013	4.8939135133	0.6543780199
H	1.5348503282	3.7092682396	1.7247566891
C	4.501423481	0.783669373	1.1883929154

H	4.3944224498	-0.2992018352	1.4003421901
H	5.1284799775	0.8746476721	0.280898903
H	5.0660256733	1.2359390773	2.0316530413
C	2.4256609643	1.3007156967	2.4105856014
H	2.2269428001	0.2315472164	2.6242927586
H	3.0651883075	1.6995226494	3.2270512775
H	1.4575225258	1.8350156244	2.4844354472
C	1.7981211171	2.0538131087	-2.605504409
H	0.7634315453	1.6577180568	-2.6544922802
H	1.8042942898	3.0291618974	-3.137154543
H	2.4351097847	1.3536694295	-3.1777433865
C	2.8943002433	-0.3075921581	-0.8431637837
O	0.8998998879	0.5570961953	0.1447614186
C	-1.9397712001	-3.0606644714	0.657389698
C	-3.009685062	-3.0586219392	1.5827200451
C	-2.2233327175	-3.2723264447	-0.7115854238
C	-4.329109848	-3.257005715	1.1481035882
H	-2.8094945306	-2.8621217828	2.6476742894
C	-3.5426575819	-3.4772669731	-1.142738873
H	-1.3967616845	-3.2889446462	-1.4377884399
C	-4.5999090589	-3.4693487851	-0.215705085
H	-5.1532855528	-3.2369906569	1.878785689
H	-3.7455718934	-3.6472790464	-2.2118448523
H	-5.635734984	-3.6270611497	-0.5559877787
Zn	-0.1579813929	-0.6495589487	-1.1482257474
C	-0.3310873146	-1.0884553068	-3.0887362464
H	-1.4114478136	-1.2942625779	-3.2696500866
H	-0.099694039	-0.1926252412	-3.7073518685
C	-1.630250206	2.836528707	1.4583968702
C	-2.5761442424	0.9640238042	0.1931170123
H	-3.2670182974	0.9136442325	1.0649138776
Zn	-0.4940527313	0.9055534973	1.6212588154
O	-1.7632015078	-0.0329951092	0.0398891506
H	-1.7426771092	3.4360771082	0.5353644624
H	-0.6576096142	3.1648564066	1.9066637147
C	-0.7800874276	0.0596705003	3.422455606
H	-1.8647666207	-0.1963345607	3.452787765
H	-0.2430607514	-0.9137195797	3.4366772042

C	-3.0770174358	1.7788630064	-0.9368848904
C	-2.3877642139	1.8541423204	-2.170246993
C	-4.2986654138	2.4828768147	-0.7992190622
C	-2.8966380633	2.6213069001	-3.2269779248
H	-1.4489440662	1.2940732188	-2.2953164094
C	-4.8069344043	3.2521840737	-1.8565073078
H	-4.8608574026	2.4096804091	0.145697017
C	-4.1059064027	3.3264640392	-3.0740022976
H	-2.3473459516	2.6676293024	-4.180678327
H	-5.7604028927	3.7903292723	-1.7340352152
H	-4.5048261518	3.9279688955	-3.9063563528
C	0.5211246161	-2.2722173957	-3.5743453352
H	1.6085081812	-2.0682442752	-3.4741433354
H	0.3278317668	-3.2017321681	-2.9924819744
H	0.3377894866	-2.5273712495	-4.6446754496
C	-0.4036103812	0.8782254617	4.6654986087
H	0.6847103997	1.1004389761	4.7085190493
H	-0.9247438614	1.860139578	4.7021221806
H	-0.6532416434	0.3555487326	5.6195556695
C	-2.7464659281	3.0836691554	2.464825451
H	-2.632258709	2.4605825716	3.3767897906
H	-2.7880199465	4.1461561254	2.8015538545
H	-3.7516405167	2.8593214054	2.0463537606
H	-3.7516405167	2.8593214054	2.0463537606

7.2.3 Additional TS

TS 0006

$E(\text{RB-P86}) = -5316.44916854 \text{ A.U.}$

First frequency = $-182.2373 \text{ cm}^{-1}$

C	2.618205329	-1.7504907397	-0.4108070733
C	3.9217758053	-0.3073680883	-1.8454498033
C	4.5635841654	-1.4104750756	-2.4269818497
C	4.2475335638	-2.706184338	-1.9987413968
C	3.2832070828	-2.858461717	-0.995556173
C	1.6322847397	-2.1828479775	0.6447698294
C	2.0990243133	-2.7017598248	1.869034419

C	1.1856756835	-3.3143400866	2.7409062302
C	-0.1543624465	-3.4258247372	2.3578539176
C	-0.5675914139	-2.8872772655	1.1167830921
H	4.216059449	0.6883265825	-2.194743355
H	5.3156909633	-1.2475938127	-3.2153331838
H	4.7377118147	-3.5884352637	-2.4389096441
H	3.0171965936	-3.8697158069	-0.6481506572
H	3.1687397014	-2.6372424067	2.1156448071
H	1.5254736856	-3.7270873296	3.7039851431
H	-0.880593413	-3.9503916731	2.9945505428
N	0.3217932949	-2.2638633839	0.3009300936
C	2.3105903746	0.8332372315	-0.1597447897
C	2.3576533778	2.1702278329	-1.0538713124
C	3.2423095195	1.2979821384	1.1234502795
C	3.75924707	2.7649528258	-0.7426155479
C	1.4687409365	3.2228811666	-0.3225435842
C	3.5636278319	2.7954480479	0.7880654446
H	3.8794168048	3.7807990971	-1.1781495533
H	4.6273515705	2.1598124783	-1.0653378486
H	1.2669671279	4.0656535838	-1.0159698775
H	0.4907763807	2.7848323442	-0.0533895292
C	2.3082284508	3.6856177724	0.9009727004
H	4.4286206639	3.1683305547	1.3761839605
H	2.5953989543	4.7545278863	0.8151083626
H	1.7779208539	3.5823402785	1.8684832633
C	4.5828230951	0.532167066	1.2317359259
H	4.427537043	-0.5504916844	1.4113301984
H	5.2154398129	0.622103003	0.3278364627
H	5.165017224	0.9333790323	2.0887522871
C	2.5320418921	1.117695714	2.4690864004
H	2.3084788961	0.0514140747	2.6700753273
H	3.1782179102	1.492596729	3.2917909027
H	1.5733310842	1.667874857	2.5446150058
C	1.9061222681	2.0388283763	-2.5102170829
H	0.848061016	1.7066880275	-2.549126889
H	1.9616242032	3.0257253936	-3.0170725451
H	2.490330539	1.3170983665	-3.1114059663
C	2.9369521067	-0.4207121352	-0.8325418342

O	0.9753962337	0.4895760171	0.1729811759
C	-1.9699220931	-3.0421363069	0.6461910933
C	-3.0492864022	-3.0293300942	1.5605228014
C	-2.2437343642	-3.2475062275	-0.7259668019
C	-4.3669056543	-3.2099678795	1.112727002
H	-2.8584410249	-2.8400897466	2.6284441355
C	-3.5611969661	-3.434050523	-1.1706748412
H	-1.4102750374	-3.2733197145	-1.4439963518
C	-4.6275067034	-3.415075996	-0.2541550209
H	-5.1975567334	-3.1823784983	1.8358056396
H	-3.7556953114	-3.5986187811	-2.2421877965
H	-5.6618755336	-3.5587302089	-0.604852504
Zn	-0.107813374	-0.6673403465	-1.1461073514
C	-0.3010368314	-1.0441700481	-3.0967100938
H	-1.3839301631	-1.2366357155	-3.2769394069
H	-0.0662148602	-0.1290637966	-3.6854977912
C	-1.6361041431	2.8460152691	1.5503736473
C	-2.5801571134	0.8687192099	0.2451416633
H	-3.2029283404	0.7964177659	1.1645134051
Zn	-0.4343516351	0.9156665208	1.604458395
O	-1.6943110916	-0.0584749841	0.0695176718
H	-0.7299115796	3.0762339843	2.1689824885
H	-2.4510313799	2.6842352632	2.2863185056
C	-0.7302414516	0.1241241602	3.4304850813
H	-1.7370800533	-0.3535362214	3.3962924631
H	-0.0072740416	-0.7090333964	3.5761814668
C	-3.2112275585	1.6031629241	-0.8631561598
C	-2.6090459053	1.7050877218	-2.1400628741
C	-4.4838360707	2.1928443115	-0.6596431342
C	-3.2611623631	2.3808799853	-3.1803861291
H	-1.6276251261	1.2371413857	-2.3096817219
C	-5.1379726545	2.8629987594	-1.7032613239
H	-4.9622382287	2.1103566546	0.3304936944
C	-4.5266820832	2.9613188134	-2.9674030519
H	-2.7812448425	2.4530640085	-4.1692742064
H	-6.1302964679	3.31015618	-1.533091371
H	-5.0379212236	3.4885608544	-3.788607409
C	0.5374429382	-2.2184249529	-3.6276720332

H	1.6272298341	-2.0308024606	-3.5224680374
H	0.3336862349	-3.166316679	-3.0804296909
H	0.3490479103	-2.4310423013	-4.7063709027
C	-0.6567478351	1.0992231565	4.6134716413
H	-1.3917218819	1.9285733553	4.5207301136
H	-0.856878036	0.6093723309	5.5963390988
H	0.3446939748	1.5761198193	4.702718338
C	-1.9069991363	4.03851861	0.6431118691
H	-2.9044962774	3.9903060837	0.1623768549
H	-1.8788323598	5.0013880516	1.2073425725
H	-1.16281108	4.1320869736	-0.1750291769
H	-1.16281108	4.1320869736	-0.1750291769

TS 0014

E(RB-P86) = -5316.44762602 A.U.

First frequency = -197.1820 cm⁻¹

C	2.595702856	-1.6050790062	-0.4938119242
C	3.8011892235	-0.1151230484	-1.963601338
C	4.3729060909	-1.2004445043	-2.6446958143
C	4.0688337938	-2.5098152391	-2.2520432381
C	3.1883231219	-2.6947651966	-1.1789085867
C	1.6732328348	-2.0682071382	0.6062139332
C	2.2005982627	-2.587344769	1.8046452388
C	1.3346982315	-3.2226380864	2.7080036004
C	-0.0165446388	-3.3584669623	2.3768961812
C	-0.4924350417	-2.8230894068	1.1559343407
H	4.0780734819	0.8899076947	-2.2990404816
H	5.0589109773	-1.0120674433	-3.4858958147
H	4.5049586566	-3.3774412509	-2.7711895132
H	2.9331834367	-3.7168935531	-0.8556529853
H	3.2783120236	-2.5074231642	2.0071373139
H	1.720647049	-3.6375808578	3.6525864595
H	-0.7026062874	-3.9067143785	3.0374985058
N	0.3519001719	-2.1730961623	0.3122841804
C	2.3134748826	0.9617676137	-0.1165447864
C	2.3755594758	2.3505202861	-0.9168116548
C	3.2898449604	1.3192462505	1.1711381268

C	3.82697258	2.8408420977	-0.6527492282
C	1.5904637727	3.4022450161	-0.0664737782
C	3.710520891	2.8046986394	0.8858491913
H	3.9939706726	3.8682873683	-1.0432090116
H	4.6355307282	2.1975488948	-1.0467600303
H	1.3554857318	4.2815415607	-0.7017480733
H	0.6221318475	2.9848480605	0.259959467
C	2.5382283973	3.7777590493	1.1052518953
H	4.6300194929	3.0814494235	1.4433993798
H	2.8963757754	4.8251584817	1.0185779489
H	2.0700258507	3.6877759596	2.1053202877
C	4.5841546774	0.4737562434	1.2317308199
H	4.3731844896	-0.6055509248	1.3634006643
H	5.2118459009	0.5716118605	0.3244808376
H	5.1952068215	0.8026577582	2.099538489
C	2.5740127365	1.1394945008	2.5142134011
H	2.314432073	0.0771528762	2.6930941759
H	3.2322187053	1.4740614377	3.3450842861
H	1.6325867167	1.7155933307	2.5945049274
C	1.8231622463	2.3395506754	-2.3445976337
H	1.9463417633	3.3408114882	-2.80979303
H	2.2890554225	1.5938727292	-3.0155316833
H	0.7353154118	2.1201845865	-2.3229794403
C	2.8992246455	-0.2611939696	-0.8813534976
O	0.9762352238	0.6123752158	0.2088277441
C	-1.9067238226	-3.0225855148	0.7395466346
C	-2.2363504594	-3.1582024434	-0.6284868344
C	-2.9415134208	-3.136147985	1.698207105
C	-3.5594632164	-3.39852401	-1.0266784488
H	-1.4407587674	-3.0883980132	-1.3845846028
C	-4.2664701563	-3.3695650979	1.2984398603
H	-2.7155869483	-3.0091250233	2.7680807966
C	-4.5806496435	-3.5038283784	-0.065676831
H	-3.792765954	-3.5068879823	-2.0975923126
H	-5.0605117546	-3.4398787292	2.0586992027
H	-5.6202554068	-3.6896616732	-0.3790196591
Zn	-0.0811671067	-0.5712989031	-1.1407758826
C	0.0670954586	-0.8218284937	-3.1216511678

H	-0.0953013608	0.1603307017	-3.6209636701
H	1.1386135565	-1.0592698122	-3.309760428
C	-1.7969493299	2.9286046153	1.1106549269
C	-2.5873217019	0.8902447736	0.1962250843
H	-3.2478244262	0.7921428788	1.0861112864
Zn	-0.4911818296	1.0326174171	1.5650708519
O	-1.6849216242	-0.0403684508	0.0545475725
H	-1.4155898333	3.3656404539	0.1642657249
H	-2.8931517649	3.0667287002	1.1034063018
C	-0.7313554604	0.3963699997	3.4539114677
H	-0.1791813114	-0.5655902268	3.5498936537
H	-0.2145989214	1.1083693381	4.1357497311
C	-3.2257129248	1.5683849123	-0.9560870191
C	-2.6317827858	1.5889349379	-2.239163458
C	-4.4833493352	2.196346443	-0.7803421048
C	-3.2748676338	2.2234010758	-3.3122936224
H	-1.6657852181	1.0848776495	-2.3943021244
C	-5.1260180866	2.8306208402	-1.8532476379
H	-4.9650231162	2.1716864102	0.2115962893
C	-4.5216546952	2.8487628778	-3.1241404491
H	-2.7999843086	2.2271745763	-4.3063214302
H	-6.1062163572	3.3097609077	-1.700367813
H	-5.0246476122	3.3463437941	-3.9686589452
C	-0.8196351494	-1.883810954	-3.7908288187
H	-0.6687870272	-1.9365343053	-4.8946360819
H	-0.6097451976	-2.9060427169	-3.4042983337
H	-1.9032465235	-1.6937930537	-3.6278901083
C	-2.1916370584	0.2151114617	3.8905902742
H	-2.7291364437	-0.5185403785	3.2507583005
H	-2.2910443245	-0.1458937782	4.9422762211
H	-2.7677570165	1.1650483996	3.8319476327
C	-1.242344041	3.6530446847	2.3511808378
H	-1.6127850811	3.2091423744	3.2985396964
H	-0.1328734776	3.6577026043	2.4099149413
H	-1.559046153	4.7243920834	2.3529895614
H	-1.559046153	4.7243920834	2.3529895614

TS 0018

E(RB-P86) = -5316.45367186 A.U.

First frequency = -197.3682 cm⁻¹

C	2.5968657226	-1.6668013674	-0.3771187999
C	3.8761170307	-0.2743139788	-1.8811201707
C	4.5342943219	-1.3926701276	-2.4120338589
C	4.239456988	-2.6715309331	-1.9221206942
C	3.2788895628	-2.7907735195	-0.9113721538
C	1.612496561	-2.0793201451	0.6889818518
C	2.0814830688	-2.538889967	1.9356738363
C	1.1848185813	-3.1807907986	2.804012629
C	-0.1360523451	-3.3870883789	2.3937247902
C	-0.5557614428	-2.8971802311	1.1346462015
H	4.152702418	0.7081086605	-2.2789906646
H	5.2819039298	-1.2552075482	-3.2094549579
H	4.7424906261	-3.5661051471	-2.3210116736
H	3.0284860979	-3.7888524299	-0.5173942568
H	3.14141696	-2.4123398679	2.1999843354
H	1.526250976	-3.5498141361	3.7840889595
H	-0.8382325787	-3.9495896306	3.02476513
N	0.3122986761	-2.2308303952	0.3283478056
C	2.2508801493	0.921013793	-0.2496599812
C	2.2390394809	2.1975616177	-1.2359688612
C	3.2003874285	1.4978615351	0.9731531705
C	3.6227434657	2.8610262158	-0.988639521
C	1.3236875739	3.2680143406	-0.5667353177
C	3.4514805863	2.9827952739	0.539159364
H	3.6959497112	3.8498717433	-1.4915489713
H	4.5082595363	2.2697845098	-1.2883685825
H	1.0940791673	4.0598173983	-1.3098752647
H	0.3613479135	2.8212601975	-0.2625486631
C	2.1622546491	3.8291364107	0.616524352
H	4.3091741772	3.4279437084	1.0863512276
H	2.4070380821	4.9016982491	0.4675299316
H	1.6484856324	3.7635667691	1.5968645896
C	4.5714129982	0.7874639359	1.0840771639
H	4.4597539756	-0.287232579	1.3325011834
H	5.1743493967	0.8435529941	0.1576352683

H	5.1635086121	1.2596500084	1.896996532
C	2.542719931	1.3733694852	2.3510605449
H	2.3500352548	0.3146918051	2.6147634701
H	3.2110057601	1.8003408225	3.1295372908
H	1.5801614718	1.9147699238	2.4370702594
C	1.7851377083	1.9572613474	-2.67728817
H	0.7347820244	1.6019767978	-2.6921481579
H	1.8198057457	2.9091791427	-3.2489746084
H	2.3839676892	1.2094101543	-3.2303893976
C	2.8952172914	-0.3547849029	-0.8604554623
O	0.9363305569	0.5635378533	0.1476445527
C	-1.9291657255	-3.1610222886	0.6259019053
C	-3.0262064903	-3.2997341202	1.5091442913
C	-2.152336356	-3.3352817929	-0.7601529408
C	-4.3089978466	-3.5886629193	1.0196354462
H	-2.8830165632	-3.1486723337	2.5900994913
C	-3.4345778067	-3.6292101131	-1.2476626014
H	-1.3045671582	-3.2544582863	-1.456005383
C	-4.5185351987	-3.7546214579	-0.3610279559
H	-5.1529102695	-3.6772570467	1.7220224759
H	-3.5860849245	-3.766143378	-2.3299674669
H	-5.5256023119	-3.9825613019	-0.7449480698
Zn	-0.1833260395	-0.6337451908	-1.1021416441
C	-0.4047013232	-1.0707280364	-3.0408428699
H	-1.4750831476	-1.3451804049	-3.1862002158
H	-0.2532046676	-0.1599708203	-3.6622941377
C	-1.4946697827	2.8875077412	1.4771625864
C	-2.5349712398	0.9793563931	0.3496180304
H	-3.1663294754	0.9577123879	1.2664291753
Zn	-0.3979922531	0.9381245359	1.6710690291
O	-1.7355128959	-0.0272482151	0.1709182274
H	-0.4687054194	3.2251159835	1.7696365865
H	-1.7199335235	3.4293387992	0.5399539136
C	-0.4940571035	0.211400211	3.5412150734
H	0.2620395455	-0.5999649505	3.6319858211
H	-0.1456663055	1.0204470194	4.2241327215
C	-3.114154715	1.761243459	-0.7656641751
C	-2.5371672617	1.76972066	-2.0573630886

C	-4.2996233395	2.5056017861	-0.5464404288
C	-3.1219844465	2.509682224	-3.0944614653
H	-1.627940378	1.1787894616	-2.2444218117
C	-4.8824919381	3.247981381	-1.5838422213
H	-4.771252183	2.488679736	0.4494314028
C	-4.2942589857	3.2541576275	-2.862119684
H	-2.6612183164	2.503525096	-4.0950162554
H	-5.806084984	3.8189902217	-1.3977881139
H	-4.7525301417	3.8340268341	-3.6791283535
C	0.5055108252	-2.1949429151	-3.5615917147
H	0.3899881142	-3.1378113122	-2.980815655
H	0.3056339346	-2.4550043357	-4.627672338
H	1.580453995	-1.9229582643	-3.4923851848
C	-1.8673856693	-0.3005079295	3.9969663726
H	-1.8564969697	-0.7186666832	5.0321191074
H	-2.6371063528	0.5015675571	3.9936702782
H	-2.2526860758	-1.1020136521	3.3307141067
C	-2.4677917806	3.2169151057	2.6012027826
H	-3.4999741176	2.8554257449	2.3941648814
H	-2.1567554011	2.7622670466	3.5648035544
H	-2.5590570552	4.3148972948	2.7748684346
H	-2.5590570552	4.3148972948	2.7748684346

7.3 27 *syn pro-R*

7.3.1 Starting TS

TS input

$E(\text{RB-P86}) = -5316.43518481 \text{ A.U.}$

First frequency = $-237.4626 \text{ cm}^{-1}$

C	-2.1138850769	-2.2674011613	-0.7269936919
C	-4.1600721462	-1.5421657992	0.3287861943
C	-4.5961297891	-2.8678373211	0.4748037649
C	-3.7917274066	-3.9192578048	0.0213556104
C	-2.5677154553	-3.6034045929	-0.5801439998
C	-0.780228898	-2.2372023046	-1.4390875791
C	-0.6941543297	-2.5075355717	-2.8200985049

C	0.5671981024	-2.7292768035	-3.393624124
C	1.7028220536	-2.7309022791	-2.5763633532
C	1.5610940864	-2.4680204732	-1.1944857253
H	-4.8352728918	-0.7558372675	0.6800094169
H	-5.5719087192	-3.0685646637	0.9451917084
H	-4.1069660218	-4.9689411669	0.1265196625
H	-1.9246790431	-4.4164685709	-0.9537543503
H	-1.608894204	-2.5665662216	-3.4263442431
H	0.6572976772	-2.9419474238	-4.4707899374
H	2.6912871787	-2.9795576356	-2.9879893394
N	0.3357937186	-2.1937753436	-0.6730713002
C	-2.4998707343	0.3116214069	-0.4284880854
C	-3.3768769245	1.3726780542	0.3989398589
C	-2.8697857383	0.7790650898	-1.9808835754
C	-4.6397941711	1.5395408223	-0.4947187167
C	-2.7701033521	2.8053206209	0.1916789482
C	-3.8662229972	1.9713492613	-1.7602066474
H	-5.3175544159	2.3344930422	-0.1142697424
H	-5.2433088036	0.6244900376	-0.6403075341
H	-3.2102138714	3.4827880446	0.9520644329
H	-1.6746824659	2.8566067617	0.3663461615
C	-3.1457056296	3.2294584611	-1.250505613
H	-4.4880187606	2.1531173014	-2.6617939623
H	-3.8382815566	4.0972613462	-1.2493421078
H	-2.2720183179	3.517724889	-1.8666143889
C	-3.6372708213	-0.2754651987	-2.8116665758
H	-3.0576280049	-1.2043322402	-2.9614280356
H	-4.6034911141	-0.5683843006	-2.3551778875
H	-3.8560050369	0.1442522407	-3.8173279261
C	-1.6014688646	1.1594229514	-2.7553576693
H	-1.0098728122	0.2563655595	-3.0066020667
H	-1.8642992918	1.6699646289	-3.7073855114
H	-0.9300375571	1.8163176309	-2.1746143868
C	-3.5262181197	1.1088945864	1.9021901132
H	-3.9557414389	0.1243352111	2.1608819577
H	-2.5303683278	1.1640635982	2.3862868253
H	-4.1649626698	1.8896604748	2.3674493315
C	-2.918326197	-1.1794775894	-0.249047181

O	-1.1205650431	0.3999829048	-0.1165100084
C	2.718161035	-2.5677266001	-0.2657423507
C	2.52413424	-3.0112605541	1.0639909439
C	4.0348070472	-2.2826410973	-0.6983731127
C	3.6134869517	-3.1571225239	1.9356542257
H	1.5095254373	-3.2595435026	1.4090197531
C	5.1224362938	-2.4249670086	0.1761973851
H	4.2106974761	-1.9081842809	-1.7178175628
C	4.9164621928	-2.8632099567	1.4963718407
H	3.4416194713	-3.5087157376	2.96512212
H	6.1374619739	-2.1801172556	-0.1739818255
H	5.7712195993	-2.9753503439	2.182214366
Zn	-0.0327044073	-0.9862537721	1.0461761099
C	-0.3528884344	-1.6502455541	2.8984360591
H	0.6060545575	-1.5714676501	3.4593430008
H	-1.0426834723	-0.9343573344	3.396813624
Zn	-0.0788717763	1.7462483435	1.0291427338
O	1.5367791392	0.2352743326	0.3149944143
C	-0.0553083577	2.077925426	3.0187429349
H	0.9382973656	1.7231660003	3.3780830401
H	-0.7931673751	1.4225542907	3.5301646313
C	2.279889371	1.286175133	0.4672739268
C	1.2348321799	3.3338721374	0.0411795548
H	0.4006821739	3.8625372604	0.5723393136
H	2.1438348045	3.7305345344	0.5342817479
H	2.4931325926	1.6526347255	1.5005845371
C	3.3783948249	1.5399120852	-0.5022234596
C	4.4899628603	2.3315769087	-0.1340314665
C	3.3366781192	0.9817793447	-1.8006904264
C	5.5364500034	2.5607231535	-1.0407273227
H	4.53478324	2.7621807151	0.880504183
C	4.3819895509	1.213569077	-2.7085280828
H	2.4661193861	0.3667962713	-2.0757707114
C	5.4852959021	2.0029141508	-2.3321371764
H	6.4002649703	3.1744011713	-0.7387715557
H	4.3365045637	0.7809162952	-3.7212993507
H	6.3051272926	2.1848441236	-3.0453929201
C	-0.921866416	-3.0738241953	3.0065720462

H	-1.0637532258	-3.4031181081	4.0630516189
H	-1.9105016367	-3.1654273973	2.5074384911
H	-0.2644859548	-3.8372771907	2.5308981638
C	-0.2713648614	3.5405129887	3.4345470633
H	-1.2736092408	3.9178323186	3.1328585612
H	-0.1982712751	3.6922078854	4.5373557262
H	0.4753138018	4.2252832698	2.975067265
C	1.1880852043	3.6647116167	-1.4421523733
H	0.2076369671	3.4150557664	-1.8976420206
H	1.360798394	4.7496041626	-1.6348873525
H	1.9614268554	3.1183931927	-2.023228151
H	1.9614268554	3.1183931927	-2.023228151

7.3.2 Lowest TS

TS 0001

E(RB-P86) = -5316.43543817 A.U.

First frequency = -217.9958 cm⁻¹

C	1.8863619598	2.3023828793	-0.6103498475
C	3.9782127384	1.6637149072	0.4070346874
C	4.3522938002	3.006223935	0.5683920072
C	3.4948455843	4.0242347358	0.1379923378
C	2.279708238	3.6568706239	-0.451147158
C	0.5390280225	2.2279389467	-1.2907064464
C	0.3981416622	2.6092494448	-2.6407445688
C	-0.8898130212	2.7967882267	-3.1663386956
C	-2.0007491407	2.6381949947	-2.3319115413
C	-1.8067399667	2.2515811989	-0.985588447
H	4.6967084548	0.9084148958	0.7375874391
H	5.3228609801	3.2457134606	1.0312910572
H	3.760517407	5.0864335451	0.2532840782
H	1.5919897291	4.442994704	-0.8017638442
H	1.2919793325	2.7847055521	-3.2559682476
H	-1.0217113466	3.102328565	-4.2165259806
H	-3.0164544496	2.8420709288	-2.6988963407
N	-0.5523555024	2.0311636723	-0.5099411786
C	2.4223229461	-0.2690621567	-0.3714157718

C	3.401716802	-1.2864195875	0.394011388
C	2.7807243019	-0.6652540824	-1.9483995689
C	4.6505573922	-1.3196937254	-0.5339483376
C	2.892648504	-2.7518785731	0.1459437941
C	3.8830751728	-1.772593514	-1.7938230791
H	5.399088003	-2.069242442	-0.1966058233
H	5.1751198284	-0.3548868344	-0.6630605165
H	3.3764742377	-3.4232437661	0.8846353038
H	1.8022616631	-2.8709984108	0.3169967672
C	3.2899817548	-3.1038038972	-1.309890335
H	4.4925322848	-1.8690235605	-2.7167393426
H	4.0620726264	-3.9012838992	-1.3383484953
H	2.4413383994	-3.4585751865	-1.9268457051
C	3.4263859261	0.4718532709	-2.7739089074
H	2.7552973593	1.3413428961	-2.8967053723
H	4.3700456115	0.8482380167	-2.3316963039
H	3.6618065102	0.0913709985	-3.7913171583
C	1.5311676967	-1.1376738333	-2.701657419
H	0.8619966386	-0.2809379962	-2.9212548994
H	1.8160747895	-1.5962105198	-3.6736411553
H	0.9344640974	-1.8705038104	-2.1307247037
C	3.577319545	-1.0688094571	1.9021616028
H	4.2877436596	-1.8164380205	2.3149684025
H	3.9401374319	-0.0658349652	2.1902409191
H	2.6070953131	-1.2195278483	2.4152593156
C	2.7498569804	1.2448474074	-0.1624538038
O	1.0614543623	-0.4711775932	-0.010668559
C	-2.9539964811	2.1415640852	-0.0468737274
C	-2.8085863622	2.523082739	1.3075421484
C	-4.2203575749	1.7000923092	-0.4983577605
C	-3.9011051362	2.4661564674	2.1851828265
H	-1.8325698655	2.8799850441	1.6695286166
C	-5.3099108312	1.6389203863	0.3835049175
H	-4.3439159438	1.3615458502	-1.5386267945
C	-5.1548850679	2.0241044403	1.7271804268
H	-3.7709035826	2.7719745996	3.2350485993
H	-6.2846479538	1.2769872734	0.0202592369
H	-6.0113506018	1.9768622722	2.4184468809

Zn	0.0308820254	0.8892711664	1.192102347
C	0.3959585354	1.5854442038	3.0221938112
H	-0.4881816452	1.3303592091	3.6495675504
H	1.2359967967	0.989750421	3.4439994525
Zn	0.1734582809	-1.9172619018	1.2353425803
O	-1.5111513581	-0.5577330672	1.0240109609
C	0.4456573999	-2.4009223666	3.170035931
H	0.945219283	-1.5632491084	3.7041181556
H	1.1481491247	-3.2645041137	3.214512402
C	-2.1870640977	-1.5753753956	0.5749637194
C	-1.0477421282	-3.6299944025	0.286559359
H	-0.4189069727	-4.1608810471	1.0391314415
H	-2.0828702801	-3.9486989224	0.5122598699
H	-2.798633003	-2.127077432	1.3265233087
C	-2.7548424946	-1.6028442347	-0.7961601988
C	-3.9614628848	-2.2990707834	-1.0396779467
C	-2.1183360714	-0.9420714645	-1.8711671302
C	-4.5277495098	-2.3224953936	-2.324123677
H	-4.4644962563	-2.815585579	-0.2049712892
C	-2.6823604142	-0.9694460501	-3.1556223836
H	-1.16162147	-0.4356127999	-1.6772602406
C	-3.8911152591	-1.6548416749	-3.3871244655
H	-5.4725791908	-2.8621581568	-2.4979937217
H	-2.1706915485	-0.4600202567	-3.9879897053
H	-4.3318253773	-1.6762082972	-4.3967367413
C	0.7211026566	3.0829419104	3.1380393584
H	1.6357201618	3.3546971297	2.5684302179
H	-0.0938764405	3.731356922	2.7417405284
H	0.8907690264	3.409910476	4.1912150868
C	-0.8777049709	-2.7447829705	3.8680738043
H	-1.5798674497	-1.8831669705	3.8588117925
H	-1.4031931391	-3.595090853	3.3793707075
H	-0.7399083897	-3.0343834014	4.936743543
C	-0.6513326149	-4.0123357541	-1.1317991914
H	0.436083801	-3.8912743711	-1.3149821126
H	-0.8923410599	-5.078669781	-1.3536828021
H	-1.1815957826	-3.40853977	-1.8990550297
H	-1.1815957826	-3.40853977	-1.8990550297

7.3.3 Additional TS

TS 0016

E(RB-P86) = -5316.43543818 A.U.

First frequency = -217.8486 cm⁻¹

C	1.8523460229	2.3512545883	-0.5759443527
C	3.9466519299	1.7100897622	0.4348103864
C	4.3119629176	3.052270032	0.6175813636
C	3.4487311182	4.0714036288	0.2016352506
C	2.2368454775	3.7055647072	-0.3951056445
C	0.5065294851	2.2788409748	-1.2595181456
C	0.3651897138	2.6800484096	-2.603725529
C	-0.9231751372	2.8674703977	-3.1283645896
C	-2.0342919484	2.6889493607	-2.2982148878
C	-1.8397906476	2.2828526345	-0.9577062732
H	4.6694160781	0.9542971145	0.7547671848
H	5.2802862902	3.2906756854	1.0857111273
H	3.7074910273	5.1333420225	0.3338187752
H	1.5446889059	4.4926764779	-0.7345990498
H	1.2587829979	2.8706503392	-3.2147831952
H	-1.05549459	3.1883250949	-4.1739218005
H	-3.0507379436	2.892001584	-2.6636021951
N	-0.5847116935	2.0631082372	-0.4835797002
C	2.4042452531	-0.2201495596	-0.3760857209
C	3.3888579422	-1.2431045478	0.3750425078
C	2.7675803041	-0.5894834923	-1.9584484265
C	4.6393142335	-1.2540908739	-0.5512709949
C	2.8894442697	-2.7077030626	0.1034129434
C	3.8766355728	-1.6921635022	-1.819289394
H	5.3920361764	-2.0040805618	-0.2243964407
H	5.157983006	-0.2841169955	-0.6645098321
H	3.3763994413	-3.3874063864	0.8323607971
H	1.799582158	-2.8363175507	0.2708548304
C	3.2911987219	-3.0344332056	-1.3570692803
H	4.4881065715	-1.770417733	-2.7425932934
H	4.0683368756	-3.8265168164	-1.3966834973
H	2.4457441406	-3.3848748059	-1.9808394804
C	3.4073769261	0.5643653978	-2.7650831186

H	4.3477857819	0.9399457939	-2.3153311354
H	3.6470776421	0.2011622981	-3.7877932113
H	2.7309022754	1.4313117936	-2.8757242177
C	1.5221879517	-1.0579093392	-2.7210319351
H	0.8478992534	-0.2020912724	-2.9281885087
H	1.8114587193	-1.4992783894	-3.6996521029
H	0.9293081071	-1.8034000237	-2.1626459584
C	3.5607031282	-1.0479062438	1.886683015
H	3.9162172836	-0.0471165142	2.1909974294
H	2.5907480005	-1.2132383776	2.3957852548
H	4.2755912273	-1.797056718	2.2888887925
C	2.7218470912	1.292369377	-0.1431055033
O	1.0441354217	-0.4364290932	-0.0207204609
C	-2.9876962315	2.150936084	-0.0226220381
C	-2.8466820417	2.512173222	1.3378067897
C	-4.2505720775	1.7085603008	-0.4829033197
C	-3.9400899855	2.4346559834	2.2127553303
H	-1.8734770765	2.8695530585	1.7068299882
C	-5.3409964301	1.6267495782	0.3962062434
H	-4.3704648988	1.3854751522	-1.5285070179
C	-5.1903748283	1.9918947627	1.7459645646
H	-3.8133562942	2.724864683	3.2674652715
H	-6.3128857913	1.2643663295	0.0258469426
H	-6.0475296759	1.9284592568	2.4350776536
Zn	0.0034039469	0.8986295396	1.2013882198
C	0.3612249483	1.568182702	3.0428032101
H	-0.5218964772	1.2970056524	3.6648351555
H	1.2048850431	0.9717285511	3.456223557
Zn	0.1632130677	-1.9072408633	1.2010494195
O	-1.529630208	-0.5550127587	1.0079415029
C	0.4355285408	-2.4193321185	3.1283831822
H	0.9286773804	-1.5868496871	3.6763610013
H	1.1436725746	-3.2788365411	3.1604935887
C	-2.1980902119	-1.5699328046	0.5419243975
C	-1.0451520063	-3.6126164583	0.2233569395
H	-0.4137851914	-4.151200662	0.9683082173
H	-2.0784652877	-3.9414719226	0.4427254971
H	-2.8071367704	-2.1373593795	1.2837632525

C	-2.7636395237	-1.5795785047	-0.8303628647
C	-3.9652758924	-2.2798103678	-1.0866969575
C	-2.1299791782	-0.897723024	-1.8938212751
C	-4.5295659979	-2.2866514296	-2.3722177388
H	-4.4660822869	-2.8127434473	-0.26102084
C	-2.6919913309	-0.9084711862	-3.1794029893
H	-1.1768966135	-0.3881397	-1.6904777018
C	-3.8958597558	-1.5980702459	-3.423553754
H	-5.4705555931	-2.8297151119	-2.5560407768
H	-2.1825310405	-0.3825596551	-4.0028253101
H	-4.334992825	-1.6063533875	-4.4340455192
C	0.6758025672	3.065871107	3.1828551684
H	0.841789593	3.3772522512	4.2413279368
H	1.5892739116	3.3529517465	2.6189498598
H	-0.1431252953	3.714850147	2.7957212638
C	-0.8866088317	-2.7828673598	3.8187364796
H	-1.5945080742	-1.9259110108	3.8217553862
H	-1.4056203092	-3.6289199646	3.3159324692
H	-0.7485711938	-3.0881969839	4.8829885982
C	-0.6445012492	-3.970133673	-1.2002674984
H	-0.8781912997	-5.0344384311	-1.4390826816
H	-1.1777750928	-3.3579345319	-1.9587229504
H	0.4423225177	-3.8390869821	-1.3800686793
H	0.4423225177	-3.8390869821	-1.3800686793

TS 0018 ¹

E(RB-P86) = -5316.43777925 A.U.

First frequency = -272.2912 cm⁻¹

C	2.1893903327	2.6399017672	-0.6754134238
C	4.5193534562	2.0601009006	-0.3843243823
C	4.8323252683	3.3848392459	-0.0431086979
C	3.8215015609	4.3564428071	-0.0100497177
C	2.5129579939	3.97682463	-0.338074317
C	0.747597915	2.4534974536	-1.0743597357
C	0.3444363216	2.8148329917	-2.3811757562

¹In this particular case, CREST change the conformation from **27** to **25**. TS 0018 is more stable than TS 0001 but do not represent the right conformation.

C	-1.0221053173	2.864501492	-2.6858800198
C	-1.9602163413	2.6123905785	-1.6755471609
C	-1.4943326075	2.295825358	-0.3773163353
H	5.336441433	1.327438015	-0.4042462626
H	5.8729685532	3.6532971674	0.2005292769
H	4.0462087972	5.3996397176	0.2626301523
H	1.7089661959	4.7310047979	-0.3354869647
H	1.1058958117	3.0643096837	-3.1341009713
H	-1.3574026606	3.1367305695	-3.6995602943
H	-3.0367489859	2.7183140363	-1.8720572237
N	-0.1703070781	2.1968446761	-0.1064857315
C	2.8189226945	0.1733634797	-1.0283387176
C	3.7363240405	-0.9352368565	-0.2907220406
C	3.1154621045	-0.1909520693	-2.608041621
C	4.9120441852	-1.1447664278	-1.2805271246
C	2.9870431042	-2.2928939309	-0.4715361199
C	4.0196771439	-1.4652562898	-2.4974731456
H	5.5587292183	-1.9998673203	-0.9834066894
H	5.5705819057	-0.2671374823	-1.4305638482
H	3.4211894534	-3.0461666637	0.2199138987
H	1.9152166448	-2.1770116503	-0.2256814973
C	3.2249468339	-2.6774642028	-1.9607403101
H	4.5572199868	-1.6727875659	-3.4477682424
H	3.8411397395	-3.5976526536	-2.0488971415
H	2.2860568285	-2.8672193297	-2.5161229316
C	3.8915416382	0.9022624423	-3.3744758218
H	4.0462878989	0.5820222607	-4.4280153098
H	3.3366373357	1.862786337	-3.3954718341
H	4.8894985516	1.1176333897	-2.9439043619
C	1.8054340542	-0.4477664913	-3.3694073939
H	1.2482208708	0.4985016107	-3.5254914824
H	2.0243621847	-0.881192456	-4.3702556956
H	1.1299525956	-1.1281758836	-2.8208543859
C	4.0624640607	-0.6802592707	1.1813622865
H	4.6303462569	-1.5367251622	1.6047292896
H	4.6585234432	0.2362863809	1.3561906279
H	3.1276219016	-0.5824110738	1.7743340578
C	3.2034488458	1.6376203558	-0.6918982919

O	1.4686089621	0.0174780435	-0.7347489271
C	-2.4405578412	2.1587595263	0.7673915208
C	-3.790704943	1.7694129521	0.5778554066
C	-2.0221718066	2.5176990033	2.0719384687
C	-4.6985682479	1.7704216159	1.6524064574
H	-4.1420455077	1.483232836	-0.4258229183
C	-2.931236333	2.5212966337	3.1406375237
H	-0.9756392255	2.8182634386	2.2258167686
C	-4.2743903488	2.1570372629	2.9355523771
H	-5.7446005609	1.4696088862	1.4829557615
H	-2.5870828468	2.8191069083	4.1435917756
H	-4.9873733805	2.1663264097	3.7746458666
Zn	0.7181491214	0.3741056222	1.0110015475
C	0.796589359	0.4193238671	2.9982993198
H	-0.2562663881	0.4282329418	3.3640638956
H	1.2092106522	-0.5583942644	3.3386542883
Zn	-2.8514431844	-1.0346259807	1.3251897011
O	-0.9952931198	-0.9249098698	0.59439874
C	-3.5804277287	-1.375597305	3.1277505597
H	-4.6885743334	-1.4152519652	3.0407118905
H	-3.345495246	-0.4784413292	3.7388135281
C	-1.4602795282	-1.2926593319	-0.5940726407
C	-3.7217596965	-1.686957559	-0.6132709899
H	-4.5099217827	-0.9489969162	-0.3243948329
H	-3.5395851049	-1.5021786597	-1.6876278161
H	-1.6112437855	-0.4909742893	-1.3500737345
C	-1.0710781296	-2.6105944479	-1.1484318628
C	-1.2087216654	-2.8758818586	-2.5308303785
C	-0.5583792682	-3.6204200434	-0.3017530838
C	-0.8469965831	-4.1255202031	-3.054983518
H	-1.5913482268	-2.0876916215	-3.2001565491
C	-0.1970803847	-4.869965312	-0.8275735065
H	-0.4349903891	-3.3994896531	0.769532478
C	-0.3425952171	-5.1269958066	-2.2035909934
H	-0.9501709563	-4.3193241039	-4.1343720443
H	0.2071946875	-5.6485580596	-0.1615280873
H	-0.0563790953	-6.1077738951	-2.6154767164
C	1.5891835817	1.568916146	3.6394072359

H	1.1977300232	2.5680298494	3.3439887799
H	1.5753608096	1.5395698931	4.7547385944
H	2.6576784643	1.5578089846	3.3338670949
C	-3.0331080314	-2.6461281942	3.7964970858
H	-1.9294145205	-2.6110284393	3.914977475
H	-3.4603274051	-2.7926996021	4.8153378481
H	-3.2679768881	-3.5659361049	3.2187071996
C	-4.1683031212	-3.1216087831	-0.3504103841
H	-4.5229914048	-3.2712765249	0.6915387116
H	-5.0025015095	-3.4236879417	-1.0248043276
H	-3.3447302273	-3.8470549021	-0.5259580368
H	-3.3447302273	-3.8470549021	-0.5259580368

7.4 28 *syn pro-S*

7.4.1 Starting TS

TS input

E(RB-P86) = -5316.45156508 A.U.

First frequency = -205.2287 cm⁻¹

C	-1.9860547676	2.2051916397	0.4809781243
C	-4.0304123563	1.6239418494	-0.6614562629
C	-4.3567331783	2.977121865	-0.837035179
C	-3.4979538486	3.970145342	-0.3523986441
C	-2.3293703255	3.570235156	0.3064788085
C	-0.681089903	2.076227771	1.2317061072
C	-0.6095413434	2.3344308052	2.6155478944
C	0.6505494835	2.4621339212	3.2207861112
C	1.8017845775	2.3912689699	2.4295665288
C	1.6737721041	2.1526833232	1.0410414127
H	-4.7444428596	0.8873161459	-1.0425305576
H	-5.2905183752	3.2460931875	-1.3560567269
H	-3.7289900529	5.0392557776	-0.4788030648
H	-1.643444105	4.33608725	0.7031278636
H	-1.5321609975	2.4575743763	3.1998260844
H	0.730020863	2.660719182	4.3014524082
H	2.7952976984	2.5687015067	2.8651066515

N	0.4463385829	1.9577059862	0.4883647092
C	-2.5400837697	-0.3396699845	0.183588259
C	-3.458988141	-1.3334255575	-0.6767530121
C	-3.0040729979	-0.7673560307	1.7200494898
C	-4.7702572133	-1.3834997293	0.1621095827
C	-3.0051743481	-2.8163754688	-0.4441523712
C	-4.0881406958	-1.8724125265	1.4614858644
H	-5.4968718226	-2.1209078496	-0.242966883
H	-5.3003606965	-0.4210155293	0.2847808656
H	-3.5172152189	-3.4443434374	-1.2020635107
H	-1.9251984111	-2.9861616348	-0.6312346263
C	-3.4518738161	-3.1898826835	0.9903866232
H	-4.7611006578	-1.9928706211	2.3362634417
H	-4.2065287227	-4.0041621453	0.9818251643
H	-2.6213419153	-3.5323323471	1.6385229812
C	-3.711908671	0.3510692636	2.5199218884
H	-3.06360878	1.2293172212	2.691771783
H	-4.6311125689	0.7213460894	2.0243525623
H	-4.005148708	-0.0445595511	3.5163354252
C	-1.8054178455	-1.2507888479	2.5486059726
H	-1.1427775586	-0.4008708088	2.8095908342
H	-2.1531587656	-1.7109691892	3.4991610779
H	-1.180981739	-1.9880314122	2.0135258098
C	-3.4933822124	-1.0721359072	-2.1881874397
H	-3.7880164399	-0.0473615073	-2.4784275029
H	-2.4824104851	-1.2479632633	-2.6112552128
H	-4.1886249649	-1.7799961352	-2.6874900658
C	-2.8476044071	1.1758064486	-0.0229322932
O	-1.1594493711	-0.5220100643	-0.0821319214
C	2.8538083508	2.2014871109	0.1381954266
C	2.7106795466	2.678998543	-1.186680136
C	4.1438661983	1.8424901896	0.595310041
C	3.8278960636	2.7975592411	-2.0263811919
H	1.7145719957	2.974228043	-1.5493359698
C	5.2586084523	1.9567702073	-0.2487460798
H	4.2755154052	1.4340428591	1.6089659142
C	5.1053313131	2.4376555147	-1.5610030895
H	3.6991816318	3.1796376536	-3.0511359306

H	6.2520234984	1.6561919075	0.1188510006
H	5.9814645633	2.5297423224	-2.2223873872
Zn	-0.0322909259	0.7871163131	-1.2674977739
C	-0.3492265785	1.505112671	-3.0979521567
H	-1.3816933102	1.2162773278	-3.3979621007
H	-0.3732706413	2.6176319085	-3.0287308855
Zn	-0.0774621028	-2.070920486	-0.9424803371
O	1.5205254573	-0.5849409194	-0.8628194648
C	0.0237671545	-2.8993788825	-2.7646766528
H	1.1147462977	-3.0454253236	-2.9313186605
H	-0.2825825742	-2.1182392395	-3.496296381
C	1.776007694	-1.1240910064	0.3057464283
C	0.8647867915	-3.274929393	0.6842141284
H	-0.2036294098	-3.602060458	0.7489402607
H	1.1370108232	-3.0012535006	1.7209287277
H	1.1878795101	-0.7786748465	1.1847983229
C	3.1613967575	-1.5610846149	0.593696749
C	3.5900393808	-1.7783551927	1.924833243
C	4.086760548	-1.7374660292	-0.4614953233
C	4.9101051074	-2.1704724321	2.1946019642
H	2.8786829524	-1.6303971697	2.7547104505
C	5.4061075045	-2.1298502554	-0.1898606359
H	3.745826645	-1.5462553368	-1.4901086709
C	5.8225096162	-2.3495079482	1.136991929
H	5.2326037219	-2.3358577734	3.2352188371
H	6.1186631948	-2.2654366934	-1.0193603239
H	6.8585186421	-2.659407984	1.348321145
C	0.6513963881	1.0633655227	-4.1788999274
H	1.6961302427	1.3475955989	-3.9259852462
H	0.6566535983	-0.0396948699	-4.3126063602
H	0.4311592685	1.5064121075	-5.1789655074
C	-0.7339681026	-4.2044896359	-3.0371527624
H	-0.5335204484	-4.6075970074	-4.0576750153
H	-0.4619950167	-5.0112538484	-2.3210580979
H	-1.8348592315	-4.0753597686	-2.9620584741
C	1.7319954403	-4.3918256361	0.1232951891
H	1.7565010905	-5.2780008397	0.799974296
H	1.369612948	-4.7439398097	-0.8641292045

H	2.7872144888	-4.0712964933	-0.0111973551
H	2.7872144888	-4.0712964933	-0.0111973551

7.4.2 Lowest TS

TS 0055

E(RB-P86) = -5316.45212862 A.U.

First frequency = -204.5866 cm⁻¹

C	-2.4904735229	-1.9357233608	-0.0408701789
C	-4.323222871	-0.7542990656	0.9908403481
C	-4.8877696602	-1.9561046846	1.4441257684
C	-4.2599119175	-3.1734113946	1.1568233029
C	-3.0737758005	-3.1460994806	0.4142317552
C	-1.224349311	-2.2155490336	-0.8153787243
C	-1.2734159842	-2.761875942	-2.1136503206
C	-0.0932001065	-3.259454931	-2.6881882114
C	1.0892483144	-3.2534875683	-1.9409003403
C	1.081396321	-2.706857591	-0.6360638706
H	-4.8640858513	0.1674786862	1.2255683755
H	-5.82480338	-1.9297391545	2.0228704261
H	-4.6803157835	-4.130800205	1.5016480942
H	-2.5648332848	-4.0934887848	0.1741279243
H	-2.2311990278	-2.8176943178	-2.6497838222
H	-0.1078193205	-3.6903622842	-3.701950774
H	2.0071865982	-3.7094842114	-2.3378323688
N	-0.0580089701	-2.1665302948	-0.1256256165
C	-2.5558637092	0.6747083583	-0.2835361531
C	-3.2170559526	1.9788262346	0.3777980751
C	-3.0478391183	0.8621549167	-1.8585375292
C	-4.5539924245	2.1121693991	-0.4105634773
C	-2.5158875246	3.2677838199	-0.1761981297
C	-3.8894408898	2.1858495349	-1.8048835409
H	-5.1009563241	3.0437672501	-0.1482465542
H	-5.2605346192	1.2678774202	-0.3094974473
H	-2.8412105735	4.1239227769	0.450761218
H	-1.4126159526	3.2541759766	-0.0710476821
C	-2.9922932979	3.4238580885	-1.6419306447

H	-4.5900275755	2.2561756133	-2.6633409038
H	-3.585977594	4.3518656374	-1.779960287
H	-2.1631169024	3.4648004435	-2.3755803999
C	-4.0013682692	-0.2397884509	-2.3766578635
H	-3.5320822719	-1.2408546454	-2.3828402408
H	-4.9314489305	-0.3236824218	-1.7805489681
H	-4.2942004269	-0.0047531376	-3.422736722
C	-1.8468705558	0.9249851647	-2.8125877752
H	-1.3663210222	-0.0705047298	-2.9016149599
H	-2.1770775928	1.2323711055	-3.8287804801
H	-1.0641381557	1.6265327273	-2.474906226
C	-3.1951403253	2.0307936374	1.9103523117
H	-3.6857644829	1.178122914	2.4136107026
H	-2.1413173525	2.0454454652	2.2573050908
H	-3.6771575138	2.9631664364	2.2737241968
C	-3.1164698504	-0.679692879	0.2512187998
O	-1.1486433058	0.6407434355	-0.115301465
C	2.2798227457	-2.7808508272	0.2405093698
C	2.1255321257	-2.9055268623	1.6420453515
C	3.5868560648	-2.7895181923	-0.3017662207
C	3.2464191219	-3.0357089351	2.4746847907
H	1.1144438267	-2.9161409911	2.0755433621
C	4.706505085	-2.917243499	0.533752878
H	3.7358154834	-2.657278648	-1.3843182547
C	4.5405012085	-3.0430387929	1.9243167979
H	3.1062250767	-3.1371254404	3.5622791468
H	5.7163369693	-2.9052536914	0.0950002956
H	5.4202262286	-3.1442582636	2.5796212689
Zn	-0.1858745491	-0.5498264002	1.3024978704
C	-0.3966996657	-0.7022961197	3.2755753175
H	0.6259179328	-0.7246343815	3.7168198316
H	-0.8515016486	0.2441768909	3.6444187244
Zn	0.2854497586	2.0939743206	0.2982323161
O	1.5617603203	0.3498939649	0.5014388006
C	0.5734584118	3.3546383977	1.8297796939
H	-0.2758964974	3.2339592028	2.5387170172
H	0.4850711818	4.3915375414	1.4316967092
C	1.8044864617	0.5511049736	-0.7727737476

C	1.2750320475	2.702451589	-1.6064750678
H	0.2779627391	3.1988904082	-1.7116079369
H	1.4207081723	2.1571516525	-2.5575831088
H	1.0858291464	0.1396048416	-1.5162703255
C	3.2137163395	0.627559701	-1.2223508578
C	3.5480392068	0.4373289557	-2.5843228002
C	4.2503696531	0.860373808	-0.2885608679
C	4.8860339598	0.4861728726	-3.0046546726
H	2.7471709354	0.2415098831	-3.3170594567
C	5.5875421644	0.9088435642	-0.7106791723
H	3.9791525692	0.9885207083	0.7701563567
C	5.910644423	0.7243485401	-2.0685502908
H	5.1340495979	0.3354184692	-4.0676571349
H	6.3872578163	1.0919404437	0.024902177
H	6.96112163	0.7650773326	-2.3984483875
C	-1.2184398245	-1.9006576857	3.7770901604
H	-0.7904197166	-2.8763901045	3.4525217229
H	-1.2864893762	-1.9449682655	4.8898972242
H	-2.2613088341	-1.8799876204	3.3934088244
C	1.9061441787	3.1745698351	2.5703094995
H	2.0252684855	3.8940401431	3.4145937723
H	2.0046708806	2.1545058408	2.9979827146
H	2.7797695206	3.3244595334	1.8996021792
C	2.3616611554	3.7345013666	-1.3463688128
H	2.5056561643	4.414749492	-2.2183182238
H	2.1256548938	4.3715512166	-0.4694253301
H	3.3483196209	3.2606504787	-1.1535371444
H	3.3483196209	3.2606504787	-1.1535371444

7.4.3 Additional TS with 28 conformation

TS 0087

E(RB-P86) = -5316.45156505 A.U.

First frequency = -205.2474 cm⁻¹

C	-2.4862020294	-1.9966488714	-0.0861528141
C	-4.3455456466	-0.783443965	0.8590340696
C	-4.9164223159	-1.9695905757	1.3443858441

C	-4.2773452132	-3.1941014158	1.1193862468
C	-3.0760357038	-3.1910992274	0.4007188308
C	-1.205364375	-2.2995392495	-0.8283571091
C	-1.2287521356	-2.8832423628	-2.1111470207
C	-0.0358876356	-3.3881656141	-2.6520495039
C	1.1328620851	-3.3561489893	-1.8843315089
C	1.0972719807	-2.7792314965	-0.5931272537
H	-4.8944715132	0.1447032275	1.0458463377
H	-5.8670239456	-1.9255245604	1.8994517768
H	-4.7024920421	-4.1392568836	1.4912516031
H	-2.5607379475	-4.1453637384	0.2052650878
H	-2.1763728788	-2.9605068124	-2.662342687
H	-0.0304190642	-3.8456005687	-3.6542043018
H	2.0601728179	-3.8176754626	-2.2522104495
N	-0.0524846306	-2.2287107599	-0.1187398567
C	-2.5382743991	0.6047583057	-0.404941893
C	-3.2240611643	1.9294335675	0.1841882641
C	-2.9621612311	0.7417710202	-2.0050874135
C	-4.5284489971	2.0322075872	-0.6605784184
C	-2.5052573603	3.2014757414	-0.3853885174
C	-3.8083197162	2.0633741082	-2.0292040205
H	-5.0887564345	2.9691481925	-0.4507591101
H	-5.2349684064	1.1877272279	-0.5599929746
H	-2.8643384788	4.0755480958	0.1960031938
H	-1.4072127296	3.2000448987	-0.2289567593
C	-2.9191235146	3.3073942587	-1.8734916662
H	-4.4741206304	2.1024783044	-2.9167857716
H	-3.5051738459	4.2301855301	-2.0674750577
H	-2.0600935495	3.3229177876	-2.5727501197
C	-3.8944998237	-0.3757508252	-2.5281480577
H	-4.8507404909	-0.4364707172	-1.9717789803
H	-4.1394502748	-0.175654492	-3.5936584841
H	-3.4302258825	-1.3773464666	-2.4791617204
C	-1.720996442	0.7788619948	-2.907927855
H	-1.240155049	-0.2193410606	-2.9520803048
H	-2.0057440655	1.061695646	-3.944831216
H	-0.9512588751	1.4870696763	-2.5533806952
C	-3.2586150397	2.040693472	1.713997142

H	-3.7325182484	1.1883174594	2.2336912535
H	-2.219549955	2.1135434976	2.0974017947
H	-3.7907459165	2.9654865346	2.0227469743
C	-3.1204777199	-0.7324373888	0.1489791806
O	-1.1402598465	0.5761132993	-0.171014566
C	2.2751869868	-2.8407390862	0.3117124425
C	2.0869707473	-2.958486758	1.7097502077
C	3.5944721217	-2.8528641183	-0.1995784715
C	3.1879677937	-3.0892654709	2.5688367658
H	1.0651883035	-2.9640564923	2.1182127562
C	4.6939932419	-2.9780555341	0.6626991268
H	3.7683680493	-2.7259779379	-1.279077413
C	4.4947721847	-3.1000219527	2.0491322452
H	3.0223026531	-3.189038697	3.6529368959
H	5.7139859411	-2.9680381346	0.2481351075
H	5.3584473422	-3.2010527709	2.725427827
Zn	-0.243740975	-0.6103075279	1.3048074002
C	-0.6318191567	-0.8053100884	3.248491492
H	-1.5801307771	-0.2609998129	3.4578980629
H	-0.8694149196	-1.8770809339	3.4432233618
Zn	0.2427633166	2.0464361434	0.3145764894
O	1.5269677429	0.3051476298	0.6089955967
C	0.5576998195	3.2427877247	1.8914409192
H	1.6613908275	3.2119978324	2.0337421683
H	0.1327503945	2.727905226	2.7822889976
C	1.8420424675	0.4968018632	-0.6501772185
C	1.3427646896	2.6329328189	-1.5373352866
H	0.3540165953	3.1341087867	-1.6919534454
H	1.5248021349	2.0773514613	-2.4764665707
H	1.1711062892	0.0745738973	-1.4308895227
C	3.2750887335	0.5806058541	-1.014264267
C	3.6939447002	0.3941978442	-2.3531730417
C	4.2506579408	0.8183565332	-0.0179822681
C	5.0549654415	0.4520188486	-2.6898950682
H	2.941052615	0.195260665	-3.1343221888
C	5.6109658496	0.876136939	-0.3565906119
H	3.9130569488	0.9420245499	1.0220054796
C	6.0183957119	0.6953491632	-1.6920640304

H	5.3692000312	0.3044421709	-3.7357050423
H	6.3626829893	1.0629603703	0.4271227876
H	7.0869686033	0.7428769955	-1.9564598901
C	0.4691421647	-0.3241531832	4.2082865783
H	1.4319195273	-0.8553887519	4.0437662644
H	0.6885714481	0.7573118597	4.0781681828
H	0.2011850845	-0.4699784464	5.2815336708
C	0.0698868333	4.6956997358	1.8384528477
H	0.3757773451	5.2801535809	2.7378885248
H	0.4664455584	5.2452266396	0.9561885198
H	-1.0373822345	4.7659004254	1.7809825084
C	2.4232432068	3.6627740397	-1.2438293491
H	2.1656198466	4.2993514067	-0.3727896396
H	3.4023267146	3.1866539848	-1.0224020118
H	2.5937983922	4.3439390503	-2.1102714111
H	2.5937983922	4.3439390503	-2.1102714111

TS 0090

E(RB-P86) = -5316.45165237 A.U.

First frequency = -199.8129 cm⁻¹

C	-2.4896298032	-2.0423920102	-0.2224052442
C	-4.39749467	-0.9211750465	0.738275435
C	-4.9406087257	-2.1411152598	1.1684276284
C	-4.2626787347	-3.3371525295	0.9068998419
C	-3.0511079136	-3.2714236414	0.2089189018
C	-1.1871569908	-2.2802668981	-0.9503318365
C	-1.1685891005	-2.8136911669	-2.254792567
C	0.0475628282	-3.2717195306	-2.7857405902
C	1.1981254684	-3.2421871211	-1.9908162495
C	1.1216010935	-2.7118736302	-0.6812992486
H	-4.9763836999	-0.0173935238	0.9516533683
H	-5.9003112232	-2.1458518801	1.7093909844
H	-4.6653842743	-4.3079030602	1.235268581
H	-2.5043941551	-4.2019327443	-0.0137758052
H	-2.1017538948	-2.8909471388	-2.8301552407
H	0.0859850798	-3.6914760783	-3.8035543634
H	2.143428555	-3.669052176	-2.3546459773

N	-0.0517661171	-2.2078780166	-0.2132190768
C	-2.6152469992	0.5667760715	-0.4458981815
C	-3.3439051869	1.8481357744	0.187739484
C	-3.0317127645	0.7532393201	-2.0428997955
C	-4.6435234261	1.9487121757	-0.6644335773
C	-2.650665962	3.1584123917	-0.32590006
C	-3.9139281088	2.0514677679	-2.0239466343
H	-5.229677316	2.8622138593	-0.4240458958
H	-5.3287462941	1.0832656637	-0.6020097174
H	-3.0236136376	4.0020137673	0.2913878044
H	-1.5533323394	3.1690381845	-0.172879134
C	-3.0634133786	3.3139292863	-1.8106979023
H	-4.5732575427	2.1065286485	-2.915545652
H	-3.6779878329	4.2249799437	-1.9689739226
H	-2.2027601003	3.3863254886	-2.5046026729
C	-3.9283429292	-0.3697337115	-2.6149461746
H	-4.1738313019	-0.1348403776	-3.6731798404
H	-3.4342782803	-1.3584321437	-2.6028072689
H	-4.8850644054	-0.4810639514	-2.0673976287
C	-1.7875284914	0.8573815196	-2.9357422055
H	-2.0759633673	1.1622997266	-3.9653420605
H	-1.042908324	1.5788677361	-2.5563520547
H	-1.2740176908	-0.1228604391	-3.0068517028
C	-3.4002532476	1.894932653	1.7196419943
H	-3.9326195265	2.8085671001	2.0596648906
H	-3.8858016946	1.0240259252	2.1959778876
H	-2.3668309263	1.9463040999	2.1203727864
C	-3.16404344	-0.8070291546	0.0502623111
O	-1.2179627594	0.5675561666	-0.2008817025
C	2.2827268472	-2.768999885	0.2455598186
C	2.0706232192	-2.9125054184	1.6378399061
C	3.6119087874	-2.7437034192	-0.2392555385
C	3.1572829854	-3.0303999045	2.5166907558
H	1.0418059422	-2.9469238771	2.0263515206
C	4.6970781537	-2.8570744095	0.6426225105
H	3.8048488832	-2.5967256097	-1.3129131036
C	4.473909268	-3.0036530193	2.0229987491
H	2.9725759524	-3.1490025326	3.5958230062

H	5.7244289381	-2.8178716398	0.2484445721
H	5.3264499382	-3.0943282353	2.7147204131
Zn	-0.3238189573	-0.6363791038	1.2544715592
C	-0.7687735471	-0.9335431542	3.1730698711
H	-1.7941659473	-0.5345301854	3.3428826242
H	-0.8620283402	-2.0330384843	3.333607493
Zn	0.1480904821	2.0528595216	0.3151910617
O	1.4440429995	0.3400656895	0.6223222175
C	0.3089910472	3.3509550692	1.8353710157
H	-0.5237934207	3.1545038308	2.5475070569
H	0.1145838919	4.3680217701	1.4239268761
C	1.7894654513	0.5532396275	-0.626712497
C	1.2322411186	2.6763364116	-1.5314280206
H	0.2236316741	3.1244138246	-1.7133103611
H	1.4641757256	2.1171284862	-2.4568919494
H	1.157413592	0.1124398008	-1.4291940686
C	3.2271302305	0.6954086213	-0.9512011325
C	3.6869520955	0.528950851	-2.2794156252
C	4.1671579195	0.9684190432	0.0697919935
C	5.0528027927	0.6399401469	-2.5813740878
H	2.9625938818	0.3024383852	-3.0798024166
C	5.5324656882	1.0780480368	-0.233911647
H	3.7998327711	1.0794966375	1.1009733993
C	5.9805385328	0.9165652519	-1.5588263767
H	5.3987501757	0.5075392354	-3.6191685138
H	6.2560904416	1.2913644795	0.5691948062
H	7.0528907035	1.0056781171	-1.7956917393
C	0.2037410673	-0.3300406286	4.1994802606
H	1.2400989382	-0.7120429875	4.0711263861
H	0.2670057805	0.7753264299	4.1075985247
H	-0.0898956498	-0.5465316217	5.2539112077
C	1.6530556276	3.3219886785	2.5768316533
H	1.8559763202	2.3260392257	3.0241982145
H	2.5073738106	3.5474567527	1.9028299912
H	1.6976175745	4.065303695	3.407563698
C	2.2534916413	3.7612985291	-1.2273675036
H	3.2416456654	3.3369708966	-0.946561486
H	2.4343692269	4.4192137987	-2.1095551435

H	1.9262839741	4.4151845731	-0.3932901262
H	1.9262839741	4.4151845731	-0.3932901262

TS 0108

E(RB-P86) = -5316.44693840 A.U.

First frequency = -211.9843 cm⁻¹

C	-2.5041820729	-1.9576654338	0.1075736588
C	-4.3491197905	-0.8135420265	1.1589311068
C	-4.9035692703	-2.0280220079	1.5864704417
C	-4.264363933	-3.2346943312	1.2740261808
C	-3.0758867536	-3.1836322811	0.5377809572
C	-1.2384364788	-2.203598751	-0.6734064946
C	-1.3256334206	-2.7160025555	-1.9844799693
C	-0.187906729	-3.2949805373	-2.5654193773
C	0.9857487722	-3.3909836302	-1.8113363148
C	1.0232015228	-2.8299385155	-0.5122558358
H	-4.8901952754	0.1021970792	1.4178473831
H	-5.8401304608	-2.0221945431	2.1665202053
H	-4.6775906626	-4.2019351876	1.5997071915
H	-2.5551869409	-4.1208827067	0.2838311184
H	-2.2896613435	-2.6970893423	-2.5133567493
H	-0.2318343926	-3.7132670963	-3.5835328456
H	1.8617326775	-3.9225112182	-2.2083436049
N	-0.0658903759	-2.2074704265	0.0114328134
C	-2.5907270144	0.6402866528	-0.0902846836
C	-3.0692733179	1.8935682321	0.8031509895
C	-3.2616172081	1.0230437291	-1.5453156671
C	-4.4467303184	2.2600509253	0.1759136867
C	-2.2569454737	3.1407477517	0.3446178728
C	-3.9089781803	2.4229618287	-1.2611755021
H	-4.8423775775	3.2116691974	0.5926951668
H	-5.2463503695	1.5015709533	0.2640736061
H	-2.4099174259	3.9540520384	1.0848225658
H	-1.1712884021	2.9325993061	0.3228049205
C	-2.8435240086	3.5174232058	-1.0435570985
H	-4.6658980444	2.685360396	-2.0302384209
H	-3.3283100717	4.5159885625	-1.0228780667

H	-2.0777511067	3.5546535958	-1.8390547763
C	-4.3833482688	0.054472512	-1.9902974926
H	-4.005200366	-0.9773066883	-2.1373032279
H	-5.2202288789	-0.0092756298	-1.2683328373
H	-4.803392573	0.3987756907	-2.9595237433
C	-2.2274652134	1.0401404818	-2.6802185086
H	-1.7938914811	0.0315771801	-2.839109149
H	-2.7105036566	1.3533684414	-3.6304306848
H	-1.3906712269	1.7465790042	-2.5045868743
C	-2.9520638249	1.744737185	2.3228563114
H	-3.4767466882	0.8676544129	2.7458632333
H	-1.8852860465	1.655380624	2.6161520723
H	-3.3527179143	2.6523050662	2.8229741895
C	-3.1446679108	-0.7211650429	0.4152448302
O	-1.1750954433	0.5134397609	-0.1346495114
C	2.2346194272	-2.9641873529	0.3450453472
C	2.1116758081	-2.948946199	1.7552148025
C	3.5223826265	-3.1469783794	-0.2184332787
C	3.2409563972	-3.1036738557	2.5737496547
H	1.1163718477	-2.8214506889	2.2042605194
C	4.6495432549	-3.3016816541	0.6027598295
H	3.6514040931	-3.1411041637	-1.311906966
C	4.5135320459	-3.2799994139	2.0027199689
H	3.1226785888	-3.0908721307	3.6686010011
H	5.6431939729	-3.4331473481	0.1459204113
H	5.3990457997	-3.39982853	2.6466820303
Zn	-0.2618318711	-0.3916026048	1.4457165879
C	-0.4091825358	-0.8283147746	3.3857916168
H	0.6335399102	-0.9555259106	3.7593052058
H	-0.788119699	0.0763125774	3.9118159135
Zn	0.3704554266	1.590212029	-1.0232782956
O	1.3058361792	0.9171543721	0.9339671861
C	0.7292495793	3.4960498399	-1.6018131361
H	1.8301124425	3.5906727342	-1.4690674381
H	0.2827336337	4.196366179	-0.8617005691
C	2.3329010377	0.5430420152	0.2282118414
C	1.7182680074	0.1999204457	-2.14771721
H	0.7222163284	-0.0366378781	-2.6033998333

H	2.1243718768	-0.7892145674	-1.8666958111
H	2.5534123028	-0.5373040377	0.1343369711
C	3.5102396307	1.425228707	0.1062119207
C	4.7186464761	0.9294726445	-0.4409474524
C	3.4723966682	2.7525831181	0.5980902998
C	5.8574748353	1.7462531647	-0.5104703804
H	4.7622241125	-0.112982024	-0.7956924723
C	4.611257129	3.5662200606	0.5261808022
H	2.539194015	3.1192783444	1.0510793238
C	5.8051303116	3.0685697969	-0.031750253
H	6.7935045254	1.3497840659	-0.9351962027
H	4.5734690544	4.5968140822	0.9138398371
H	6.6992016628	3.7101746907	-0.085034168
C	-1.2624585521	-2.0465760459	3.7667017893
H	-0.9123159412	-2.9808834979	3.2722589243
H	-1.2627944964	-2.2511447762	4.8634508599
H	-2.3236725206	-1.9210809761	3.4625125774
C	0.3677164191	3.9481472856	-3.026160095
H	0.7135861262	4.986784543	-3.2396418928
H	0.8214939702	3.3009288651	-3.8075667054
H	-0.7269351513	3.9414832669	-3.2197339901
C	2.6221076855	0.9107332789	-3.1430140141
H	2.9024355692	0.2564575997	-4.003129228
H	2.1499559872	1.8191020949	-3.5668107926
H	3.5782021725	1.2375551765	-2.6779469716
H	3.5782021725	1.2375551765	-2.6779469716

TS 0124

E(RB-P86) = -5316.44658822 A.U.

First frequency = -190.1436 cm^{-1}

C	-2.4551339098	-1.9638153717	-0.082749765
C	-4.2989930603	-0.8773229641	1.0266358782
C	-4.8280212073	-2.1115289239	1.4309262827
C	-4.1811518835	-3.2996649855	1.0706489463
C	-3.0038793934	-3.2091135762	0.3201142921
C	-1.1678806281	-2.1775433455	-0.8390708285
C	-1.1761770675	-2.6820196737	-2.1543365498

C	0.0134386665	-3.2022567309	-2.6883533845
C	1.1590487225	-3.2543719729	-1.8875817594
C	1.1166652103	-2.7163088562	-0.5785805891
H	-4.851706573	0.0196183669	1.3208955174
H	-5.7527517396	-2.1341452327	2.0292146016
H	-4.5764371597	-4.2819507935	1.372513609
H	-2.4714950924	-4.1309801036	0.0357746055
H	-2.1138713259	-2.700953784	-2.7280665048
H	0.0318842811	-3.611188285	-3.7110221218
H	2.0742620874	-3.7412692252	-2.2525261171
N	-0.0261833774	-2.1504556209	-0.1053062224
C	-2.6134194213	0.6429180464	-0.248805742
C	-3.2502313477	1.8907070278	0.5360918836
C	-3.2279112811	0.9020202392	-1.7660177364
C	-4.6375760421	2.0554588525	-0.155334813
C	-2.58665186	3.2070414499	0.0217518101
C	-4.0658201041	2.2152570979	-1.5815735633
H	-5.1641926245	2.9687522464	0.1973016624
H	-5.3399891509	1.2070823622	-0.0617231623
H	-2.8663830277	4.0284253729	0.7139624552
H	-1.4833536485	3.1529932202	0.051066401
C	-3.1599153946	3.4470712408	-1.398982174
H	-4.8198424291	2.3314076278	-2.3884299357
H	-3.7657884137	4.376266887	-1.4435198694
H	-2.3787078738	3.5426003848	-2.1792173953
C	-4.197045337	-0.1966145572	-2.2622415402
H	-3.7030865585	-1.1836172887	-2.35341655
H	-5.0743982252	-0.3349934386	-1.6007189292
H	-4.5769764737	0.0799433564	-3.2692070437
C	-2.1167802951	1.0267405636	-2.8133297662
H	-1.6018416547	0.0563744384	-2.9584668459
H	-2.5419709985	1.3377030459	-3.7919626063
H	-1.3417071293	1.7646222013	-2.5365453943
C	-3.1396471825	1.853192497	2.0645806011
H	-3.6490946258	2.7352738242	2.5075871257
H	-3.5557402466	0.9470077968	2.5422278025
H	-2.0708263397	1.9077341514	2.3587706899
C	-3.1113462474	-0.7417139515	0.2630649183

O	-1.1897507824	0.6129095359	-0.1916798832
C	2.2806453111	-2.8231866012	0.3434460819
C	2.07608714	-2.8687554742	1.7430304233
C	3.6042173253	-2.9258100139	-0.1494507944
C	3.1617495826	-3.0115423113	2.6199150737
H	1.0526866196	-2.8051469751	2.1404309471
C	4.6884181559	-3.0660155873	0.7290839617
H	3.7958580455	-2.866665665	-1.2320270305
C	4.4710026365	-3.1107372654	2.1177268647
H	2.9805311174	-3.0486036939	3.7055006943
H	5.7115669342	-3.1281581159	0.3267313273
H	5.3228536889	-3.2190799153	2.8075659747
Zn	-0.239827335	-0.4705764867	1.3064974472
C	-0.4731908756	-0.6825476585	3.2738464672
H	0.5497734491	-0.7317706895	3.7132251797
H	-0.9123214308	0.2585987042	3.6737017801
Zn	0.3272786798	1.9804738665	-0.4900283762
O	1.4975256852	0.5260318332	0.668153261
C	0.8475819742	3.826900326	0.1240897515
H	0.296983936	4.5698505821	-0.497337243
H	1.9153768122	3.9246577384	-0.1757882886
C	2.2344101656	0.408841071	-0.4024870891
C	1.503860062	1.6363421337	-2.3758994251
H	2.4565735705	2.1984435268	-2.3629505517
H	0.7232000971	2.376497421	-2.6808418215
H	2.0597628406	-0.4428093804	-1.0909827519
C	3.61347254	0.9505115695	-0.3721379926
C	4.5659306761	0.5949928086	-1.3576380235
C	4.0061238717	1.8178884026	0.6751377619
C	5.8707440531	1.1071017707	-1.3076911557
H	4.2783137388	-0.0916773998	-2.1697049951
C	5.3114776195	2.3274324419	0.7239231343
H	3.2660666708	2.072497445	1.448024504
C	6.2475351935	1.9778452825	-0.2677520457
H	6.6017758216	0.8228635907	-2.0815467663
H	5.6046530348	3.0027686078	1.5436484805
H	7.2726685995	2.3796268878	-0.2279597651
C	-1.3103961807	-1.882940024	3.7421619806

H	-2.3526681539	-1.8374962275	3.3591605466
H	-0.8964140768	-2.8544567523	3.3882983491
H	-1.3787606716	-1.958400437	4.8532479958
C	0.6890579838	4.1512376133	1.6149251212
H	1.038483588	5.1792532456	1.8723495482
H	-0.3692571381	4.0864599322	1.9501361598
H	1.2632466622	3.448758891	2.2573566687
C	1.4954381234	0.476664025	-3.3594565381
H	2.3458983582	-0.2226089718	-3.2067960094
H	0.567886415	-0.1284305523	-3.2810889208
H	1.5670481123	0.8196225815	-4.4185697522
H	1.5670481123	0.8196225815	-4.4185697522

TS 0131

E(RB-P86) = -5316.44696622 A.U.

First frequency = -200.9142 cm⁻¹

C	-2.4525419368	-1.9599651974	-0.0176646267
C	-4.2923708661	-0.7663983328	0.9876554044
C	-4.8546522083	-1.9621698635	1.4592558267
C	-4.224627721	-3.1827478442	1.1908167079
C	-3.03462963	-3.1644226384	0.4542459926
C	-1.1690654825	-2.2470391692	-0.7601983754
C	-1.1811097027	-2.8213800042	-2.0467768347
C	0.0150237829	-3.3342901073	-2.5735501046
C	1.1744838973	-3.3148249474	-1.7910190921
C	1.130421254	-2.7350794371	-0.5009232242
H	-4.8343189133	0.1579048592	1.2093483989
H	-5.7919227469	-1.9286134252	2.0372156571
H	-4.6446846959	-4.1355379287	1.5485590619
H	-2.520365263	-4.113890843	0.2345930937
H	-2.1226734399	-2.88836677	-2.6097996694
H	0.0297427107	-3.7887489239	-3.5769742578
H	2.101103407	-3.7854475533	-2.1489203554
N	-0.0222125645	-2.179588583	-0.0395238187
C	-2.534556021	0.6409249462	-0.323709479
C	-3.2007052094	1.9577682759	0.3035238915
C	-3.0307168898	0.7845604642	-1.9005992013

C	-4.5440248466	2.0569285935	-0.4794148785
C	-2.5110228655	3.233762362	-0.2935950344
C	-3.8895289612	2.0986154502	-1.8791700964
H	-5.0976710747	2.9904402314	-0.2388328942
H	-5.2421598212	1.2095520289	-0.3507409563
H	-2.8262475113	4.1056663262	0.3163680059
H	-1.4060308206	3.218128663	-0.2033180114
C	-3.00666199	3.3512130413	-1.7562831433
H	-4.5959670847	2.1355804609	-2.7348704849
H	-3.6151464152	4.2675608576	-1.9071700487
H	-2.1864754646	3.3870709076	-2.4996213369
C	-3.9647922291	-0.3427413701	-2.397592469
H	-3.4815823498	-1.3372237193	-2.376874397
H	-4.8975605162	-0.4250407739	-1.8052661687
H	-4.2542226746	-0.1367614004	-3.4507138209
C	-1.8243610681	0.8475400139	-2.8445268478
H	-2.1430966336	1.1454877961	-3.8670565949
H	-1.0539570841	1.5581405016	-2.4959583156
H	-1.3303306796	-0.1424878168	-2.9174969394
C	-3.1701908546	2.0542375852	1.8335400441
H	-3.6671489953	2.9877829701	2.1730591326
H	-3.6423856313	1.2071731134	2.3635017193
H	-2.1149235347	2.0979129012	2.1733706884
C	-3.0859369274	-0.7017771588	0.2464440714
O	-1.1245244576	0.6136033945	-0.1599610304
C	2.3004668677	-2.7873072439	0.4149472511
C	2.101885313	-2.8508784251	1.8150283419
C	3.6240800671	-2.8302605917	-0.0839980245
C	3.1950953777	-2.951619745	2.6875715025
H	1.0779827745	-2.8361910758	2.2169097853
C	4.7162691937	-2.9262144461	0.7909287956
H	3.8091753721	-2.750365055	-1.1658463487
C	4.5057696423	-2.988961308	2.1797033479
H	3.0197685634	-3.0049435881	3.7734808757
H	5.7393490971	-2.9386772499	0.384175186
H	5.3638445355	-3.0646379895	2.8663668448
Zn	-0.1951930831	-0.516490453	1.3292325289
C	-0.4396570694	-0.5884633613	3.3030421672

H	0.5772765797	-0.5912477195	3.7578020381
H	-0.8979528645	0.3735667948	3.6241208533
Zn	0.3004949487	2.0804263486	0.1839040211
O	1.5722696645	0.3666588159	0.5648782425
C	0.6124969597	3.39606893	1.6724409738
H	1.5534525759	3.068134538	2.1673367377
H	-0.1876018384	3.2693399242	2.4353419273
C	1.9719846584	0.5151874592	-0.6726813749
C	1.5366474092	2.7171065655	-1.5794674386
H	2.4847774041	3.1027531339	-1.1555638399
H	0.7824367155	3.5315351979	-1.4365075051
H	1.363367569	0.0751490171	-1.4954471417
C	3.4307312593	0.6088855674	-0.9207724856
C	3.9946824967	0.1622109916	-2.1395006097
C	4.2928838486	1.0908683277	0.0933914733
C	5.3827296112	0.2197928146	-2.3503460444
H	3.3382999868	-0.2584116433	-2.9185848566
C	5.6763398216	1.1515552357	-0.1198630069
H	3.8498136415	1.408662707	1.0492904723
C	6.2270067015	0.7208796158	-1.3436411965
H	5.8082619517	-0.1331226259	-3.3035438218
H	6.3363432605	1.5355613611	0.6745519325
H	7.3151969454	0.7707052761	-1.5089844566
C	-1.2693182458	-1.7633476801	3.8447913775
H	-0.8363245585	-2.7524786015	3.5714759186
H	-1.3551284631	-1.7575484976	4.9572431622
H	-2.3059631162	-1.7606857423	3.4439463803
C	0.7179824233	4.8651660069	1.2468440922
H	1.5378971218	5.0325695649	0.514169046
H	-0.2154829068	5.2349111947	0.7667265755
H	0.9192815052	5.5487848126	2.1052885897
C	1.6289057207	2.4148619307	-3.0659982677
H	0.6844154971	1.9998095396	-3.4755851111
H	1.8531135489	3.3340634664	-3.6564077062
H	2.4390889579	1.6967891454	-3.3062297368
H	2.4390889579	1.6967891454	-3.3062297368

7.4.4 Additional TS with 26 conformation²

TS 0001

E(RB-P86) = -5316.45414117 A.U.

First frequency = -194.1627 cm⁻¹

C	-2.5910527288	-1.6555247413	0.5525310278
C	-3.9625429561	-0.0419253154	1.7161412131
C	-4.638462474	-1.0599043401	2.4037636576
C	-4.3048958871	-2.3995675255	2.1672973358
C	-3.2916215032	-2.6785167918	1.243167827
C	-1.559506924	-2.2317978691	-0.384557564
C	-1.9817316365	-2.9439051206	-1.525842253
C	-1.0432531156	-3.7006030976	-2.2438392904
C	0.280530177	-3.7485618116	-1.7960454919
C	0.6528862532	-3.001067635	-0.6540461998
H	-4.2716555228	0.9898514269	1.9150331272
H	-5.4304451803	-0.7964870308	3.1228357055
H	-4.8197266846	-3.2182424452	2.6937038776
H	-3.012624393	-3.7260274767	1.0460865685
H	-3.040555729	-2.9179469417	-1.8218429304
H	-1.3509948241	-4.2705469819	-3.1348092308
H	1.0267641406	-4.3751799578	-2.3045742313
N	-0.2619523617	-2.2517346725	0.0142985755
C	-2.2605358207	0.880328367	-0.009650445
C	-2.3319028086	2.3137511123	0.7266491113
C	-3.1320245287	1.2007348751	-1.3739500956
C	-3.7056930086	2.884657942	0.2767735507
C	-1.3893515125	3.2686336875	-0.0691444908
C	-3.4351144847	2.7323372329	-1.2343847816
H	-3.827257514	3.9460913146	0.5844291063
H	-4.6002019975	2.3339158913	0.623875467
H	-1.219645619	4.1872369181	0.5302200888
H	-0.4022745818	2.7998248918	-0.2270907761
C	-2.1567234039	3.5854421069	-1.3841325505

²An inversion of the two ethyl groups is observed at the reactive Zn centre during the CREST process. Following the application of DFT optimisation, some TSs were observed to adopt a conformation corresponding to **26**.

H	-4.261511109	3.0477406049	-1.9057959813
H	-2.4274205497	4.6602887479	-1.4467303155
H	-1.5788235114	3.3586385352	-2.3024678653
C	-4.4801109365	0.4439740125	-1.4453038576
H	-5.0231752902	0.7483542571	-2.3655449622
H	-4.333986091	-0.6539942162	-1.4910748837
H	-5.1452815291	0.6455557725	-0.5839473076
C	-2.3727295102	0.8467071369	-2.6563367279
H	-1.4180411229	1.3970994279	-2.774083219
H	-2.1352395576	-0.2348361399	-2.7026293797
H	-2.990256367	1.0995561937	-3.5448095804
C	-1.9677797569	2.3471759316	2.2126573437
H	-0.924686599	1.9989404295	2.3560465834
H	-2.0239237575	3.3889585787	2.5941484846
H	-2.6063385757	1.7163685763	2.858982798
C	-2.9250307342	-0.2827420359	0.7805740809
O	-0.918176102	0.4952074254	-0.2531505347
C	2.0414031515	-3.0606458595	-0.1247864716
C	3.1470465422	-3.1585181005	-1.0016791471
C	2.2757385626	-3.0594354302	1.2696274202
C	4.4530412968	-3.2465311212	-0.4959607074
H	2.9842576332	-3.1272966898	-2.0904103327
C	3.5819592233	-3.1544337252	1.7728928869
H	1.4215402732	-2.9970388919	1.9605061007
C	4.6748505897	-3.2471672199	0.8929950576
H	5.304930096	-3.3063173733	-1.1918579433
H	3.7465748286	-3.1587658024	2.8619053302
H	5.7002272762	-3.3183401777	1.2894002471
Zn	0.121116266	-0.4721890769	1.2404878197
C	0.2290681293	-0.615842422	3.2294234514
H	1.3067522926	-0.7562090889	3.4767257348
H	-0.0520491829	0.3526414507	3.7003275533
Zn	0.5232299253	0.6711765186	-1.7146336833
O	1.7543248472	0.0179755559	0.0318345151
C	0.9053123695	-0.4193681891	-3.3597523522
H	0.3977018978	-1.4022734094	-3.2487553101
H	1.9972955347	-0.6394481442	-3.3136491444
C	2.5441259331	1.0087681129	-0.238164748

C	1.5964942411	2.642756987	-1.7985857686
H	1.6550175986	3.3743904654	-0.9707109175
H	0.6335630893	2.8687635705	-2.3243624479
H	3.2702054179	0.854795505	-1.0682146455
C	2.9762893106	1.9968843164	0.7760103377
C	4.181958536	2.7141937921	0.5789260886
C	2.2366305188	2.2286408592	1.9596974209
C	4.6256698845	3.646963202	1.5281832957
H	4.7831849546	2.5224106199	-0.3244175876
C	2.6810274139	3.1592329382	2.9087378752
H	1.309883854	1.6613674191	2.1330332329
C	3.8748993492	3.8750236727	2.6959090798
H	5.5675845468	4.1934152385	1.3611875444
H	2.0931180434	3.3261383713	3.8252072284
H	4.2231128994	4.6052239178	3.4437810386
C	-0.6079883813	-1.7437827245	3.8542847572
H	-1.6958406305	-1.5937062011	3.6866579977
H	-0.3653438105	-2.7414922503	3.4234472829
H	-0.460408531	-1.8328215215	4.9563795329
C	0.5552492983	0.1944604867	-4.7226866663
H	-0.5364427502	0.3704023998	-4.8363761457
H	1.0489148315	1.1776987123	-4.885826236
H	0.8576803903	-0.453674483	-5.5795349515
C	2.7444694387	2.7776542866	-2.7904875433
H	2.7693363249	3.7802492087	-3.2785204586
H	3.7381247612	2.6510793828	-2.3083519184
H	2.6843455563	2.0243618343	-3.6040567166
H	2.6843455563	2.0243618343	-3.6040567166

TS 0038

E(RB-P86) = -5316.45230478 A.U.

First frequency = -187.9422 cm⁻¹

C	-2.5661365043	-1.6837324667	0.475592425
C	-3.9698842622	-0.1655030034	1.7252137328
C	-4.584440213	-1.2320731207	2.3962776833
C	-4.1973269861	-2.5483150646	2.1134630282
C	-3.2002950377	-2.7567054286	1.1534506417

C	-1.5456547606	-2.1870302874	-0.5161122074
C	-1.9756748107	-2.8004496406	-1.7097483435
C	-1.0441581801	-3.5145659524	-2.4792755861
C	0.2711512823	-3.6370087741	-2.0207067138
C	0.6500354449	-2.9929944669	-0.819067092
H	-4.3146334115	0.8463114519	1.965024695
H	-5.3689685526	-1.0253722881	3.141598587
H	-4.6618678137	-3.4033495763	2.6288956486
H	-2.8856412247	-3.7850542947	0.9131790419
H	-3.0327483666	-2.7367113568	-2.006128391
H	-1.354110019	-4.0050388819	-3.415603361
H	0.999634473	-4.2520875912	-2.5671127375
N	-0.2512237053	-2.2588049237	-0.1149858248
C	-2.3153896108	0.874243174	0.0153789861
C	-2.4019004476	2.2700824901	0.8205280529
C	-3.2125431249	1.2448004073	-1.3202813259
C	-3.7920723435	2.8358536128	0.4181372564
C	-1.4880367339	3.2785240447	0.0589278286
C	-3.541180107	2.7617513147	-1.1018585095
H	-3.9287443685	3.8785204377	0.7790881263
H	-4.6704108597	2.2513421088	0.7509266132
H	-1.3243921623	4.1703634573	0.6990057914
H	-0.4965144366	2.8347188561	-0.1361230167
C	-2.280562708	3.6443324301	-1.2279499758
H	-4.3826986203	3.0936772788	-1.745978816
H	-2.5707417372	4.7159143451	-1.234448916
H	-1.7127076424	3.4727180341	-2.1645204865
C	-4.5485681069	0.467504983	-1.4035064992
H	-5.1124515077	0.8023687392	-2.3003666131
H	-4.3844552664	-0.6245661071	-1.5002306012
H	-5.2027536352	0.6181283429	-0.5234701219
C	-2.4748145364	0.9701315987	-2.6346223102
H	-2.2350761413	-0.1054087797	-2.7490337901
H	-3.1112719103	1.2687437781	-3.4953200477
H	-1.5258253814	1.5316498501	-2.7403531122
C	-2.0208059089	2.2404282556	2.3019085286
H	-2.0689547049	3.2655474669	2.7269635734
H	-2.6565965347	1.5861811755	2.9273156586

H	-0.9777702274	1.8816340688	2.4190238872
C	-2.9446656371	-0.3354258259	0.7614299441
O	-0.9678152325	0.5215408758	-0.2565315935
C	2.0136586326	-3.1715020877	-0.2497373243
C	3.1311642394	-3.4255403484	-1.0804724733
C	2.2049194758	-3.1574066504	1.1520660472
C	4.4020692576	-3.6440908181	-0.5273253361
H	3.0138966934	-3.4239323935	-2.1748421256
C	3.4747981475	-3.3846198238	1.7037536296
H	1.3405734016	-2.9828067053	1.8098047164
C	4.5791091968	-3.6257189752	0.8674433234
H	5.2616410248	-3.8246263888	-1.1921082596
H	3.6008977001	-3.3786693319	2.7978714612
H	5.5760992929	-3.8008860948	1.3019693763
Zn	0.1143104015	-0.4965737423	1.1864614661
C	0.0247914344	-0.8323190571	3.1566890916
H	-0.7756934365	-0.1930142899	3.5899820483
H	-0.3750719872	-1.8707228915	3.2349278141
Zn	0.439113199	0.7533843066	-1.7359000654
O	1.715259448	0.0496110265	-0.0338165073
C	0.6818684055	-0.1964365363	-3.4887036864
H	0.3444221104	0.5048024413	-4.28667855
H	-0.0338510714	-1.0476551651	-3.5182098643
C	2.4663610709	1.0780097687	-0.2886563551
C	1.4502597876	2.7570229346	-1.7550745275
H	1.5583732931	3.4379700265	-0.8908727228
H	0.4467090588	2.9914360956	-2.1912587117
H	3.1883910832	0.9672707356	-1.1289145913
C	2.8780778068	2.0575923196	0.7410873966
C	4.07235847	2.7962139123	0.5555799161
C	2.1204691151	2.2771252303	1.9149176691
C	4.4917102307	3.7328412427	1.5122369255
H	4.6817121701	2.6197547951	-0.345631086
C	2.5387462512	3.2136054497	2.8700439999
H	1.1966640463	1.6988734034	2.0715766521
C	3.7249234279	3.9465248501	2.6722240095
H	5.4261272841	4.295129903	1.356229393
H	1.9362236162	3.373287301	3.7782518629

H	4.0531298491	4.6808977052	3.4249608194
C	1.3021798479	-0.7052660086	4.0016757492
H	1.6982066299	0.3325529402	4.0163315508
H	1.1419711093	-0.9974643452	5.0661251184
H	2.1296862477	-1.3408106016	3.6181947929
C	2.1006678246	-0.6944222932	-3.7963775263
H	2.8334810206	0.1388584621	-3.8619073708
H	2.4804584336	-1.3775882717	-3.0070199878
H	2.1693555396	-1.2472681755	-4.7639754819
C	2.5180408716	2.9762170167	-2.8175371453
H	2.5689323879	4.039031012	-3.1517863217
H	3.5396475875	2.7225877238	-2.4560126858
H	2.3345166647	2.361445033	-3.7231154836
H	2.3345166647	2.361445033	-3.7231154836

TS 0040

E(RB-P86) = -5316.44916851 A.U.

First frequency = -182.0765 cm⁻¹

C	-2.5815094557	-1.7747005607	0.563059372
C	-3.9870584702	-0.1900366256	1.7264019079
C	-4.6181895644	-1.2215070231	2.4368122298
C	-4.2449996843	-2.5526983165	2.2114181236
C	-3.2357574227	-2.8113642087	1.2765308797
C	-1.5400008489	-2.3170489777	-0.3826315087
C	-1.9395563733	-3.0215448284	-1.5358768791
C	-0.9725470409	-3.7184621516	-2.2767039788
C	0.3532754804	-3.7256361201	-1.8328446387
C	0.6980663787	-3.0013389467	-0.6677018019
H	-4.3259926261	0.8339431723	1.9177378374
H	-5.4069408705	-0.9752884922	3.1654688903
H	-4.7256251505	-3.3803658843	2.7558027918
H	-2.924648382	-3.8514874662	1.0882697921
H	-2.9996228625	-3.0316273639	-1.8281564606
H	-1.2593743597	-4.2761366893	-3.1822833607
H	1.1209667582	-4.3088177985	-2.3605883705
N	-0.2430116089	-2.3007757555	0.0170176386
C	-2.3432183848	0.756262942	-0.0458319919

C	-2.4680771452	2.2044457066	0.6443836781
C	-3.2349527554	0.9992914806	-1.4156535785
C	-3.8731353854	2.6976310543	0.1998253813
C	-1.5823440258	3.1736335838	-0.1977562917
C	-3.6154497678	2.5166634804	-1.3111436795
H	-4.0421889004	3.7601711998	0.4800109428
H	-4.7349355139	2.1136809372	0.5743286318
H	-1.4355050302	4.1134320984	0.3741169624
H	-0.5810513899	2.7375462218	-0.36506253
C	-2.3842071588	3.426411316	-1.5050361655
H	-4.4663808787	2.7703881703	-1.9779849098
H	-2.7071460292	4.4855578425	-1.5845696205
H	-1.8114087619	3.2053393326	-2.4275303872
C	-4.5458169325	0.1778816122	-1.4614373214
H	-5.1041151929	0.4314649307	-2.387935115
H	-4.3502267672	-0.9129899884	-1.4775806703
H	-5.2176789609	0.3728461598	-0.6035816408
C	-2.4645979594	0.6548205141	-2.6945674652
H	-3.0872779508	0.8854263481	-3.585650163
H	-1.5206158434	1.2225658472	-2.8132473577
H	-2.2008283022	-0.4205218511	-2.7320062527
C	-2.0733466713	2.2983812979	2.1200027403
H	-2.1799310935	3.3447822881	2.477262928
H	-2.6595783272	1.6490429426	2.7969925641
H	-1.0081333475	2.0137030849	2.2449374374
C	-2.9581327617	-0.4108380069	0.7770491292
O	-0.9855327766	0.4172269136	-0.2767825743
C	2.0837507232	-3.0368385729	-0.1286388506
C	3.1992151839	-3.1153842353	-0.9951049982
C	2.3065506528	-3.0347516463	1.2679016584
C	4.5020193506	-3.1827828267	-0.4779707639
H	3.0471456937	-3.0871043188	-2.0854097566
C	3.609507755	-3.1084425234	1.7828251441
H	1.4451990335	-2.9881366347	1.9511186125
C	4.7118359439	-3.1816886885	0.9128295059
H	5.360717334	-3.2284592527	-1.1665465438
H	3.7643254524	-3.1116712196	2.8732719618
H	5.7346656014	-3.2365516145	1.3182349277

Zn	0.0772044666	-0.4995040341	1.2338316951
C	0.2013263082	-0.5870395669	3.2240922003
H	1.2811645032	-0.7134202169	3.4693742352
H	-0.0845932001	0.3938351204	3.6661022935
Zn	0.4685471336	0.6863978621	-1.7020951815
O	1.6932786313	-0.0134021653	0.0019441697
C	0.8639056784	-0.3459683181	-3.3833025374
H	0.173439055	-1.2170270755	-3.4340523871
H	1.8826112992	-0.7770958301	-3.2439252523
C	2.5570177922	0.9104651876	-0.2730142455
C	1.6073271489	2.6469337349	-1.8819099016
H	0.7209711542	2.7538892504	-2.5600081153
H	2.4566338703	2.4118423552	-2.5566809061
H	3.218522217	0.7305344231	-1.1495767259
C	3.1198522979	1.8173700843	0.7402453139
C	4.3809573688	2.4177608477	0.4998029081
C	2.4635376766	2.0780296463	1.9669580234
C	4.9713621253	3.2527688621	1.4591415062
H	4.9013959002	2.2126715485	-0.4505256492
C	3.0518856518	2.9180763971	2.9221435932
H	1.490869538	1.6037736332	2.1667828018
C	4.3065907069	3.5077169624	2.6734207862
H	5.9555671592	3.7067931994	1.2621248903
H	2.5302776102	3.1127928973	3.8726393569
H	4.7676843248	4.1645623762	3.4281874943
C	-0.6228693137	-1.7024388797	3.8877365656
H	-0.4724916285	-1.7522949919	4.9919060899
H	-1.7125398616	-1.5703081435	3.7172569124
H	-0.3688112512	-2.7108770117	3.4902575266
C	0.8096818931	0.4473247682	-4.6960923966
H	-0.2014869744	0.8695397963	-4.8898713062
H	1.5140240328	1.3078567954	-4.6964992998
H	1.0658262748	-0.1698444234	-5.5902556275
C	1.8036694866	3.9653517554	-1.1458506354
H	2.7807115111	4.0216203499	-0.625586721
H	1.7710213298	4.8364193664	-1.8433082357
H	1.0227088457	4.1479513655	-0.3786049302
H	1.0227088457	4.1479513655	-0.3786049302

TS 0063

E(RB-P86) = -5316.44695238 A.U.

First frequency = -189.4163 cm⁻¹

C	-2.5745364722	-1.7139921393	0.6950601426
C	-3.8594416694	-0.0173446855	1.8410839354
C	-4.3833872265	-0.9708900996	2.7277810805
C	-4.0167110663	-2.3161366338	2.6028099778
C	-3.1218924416	-2.6704460687	1.5848730236
C	-1.6264755874	-2.3405267137	-0.298649505
C	-2.1112903512	-3.1378802369	-1.3541578849
C	-1.1953784292	-3.8478713111	-2.1461225788
C	0.1668591579	-3.7863402562	-1.8365777108
C	0.5934300236	-2.9972073232	-0.7423543302
H	-4.1942161915	1.0182767622	1.9617394142
H	-5.0846783108	-0.6514656855	3.5150749737
H	-4.4165420613	-3.082512829	3.2849234448
H	-2.8192663999	-3.7238666595	1.4704501658
H	-3.1927825835	-3.2023022825	-1.5405310177
H	-1.5486413557	-4.4703328759	-2.9834777529
H	0.9005961519	-4.3782048317	-2.4022136502
N	-0.3010975836	-2.2755446101	-0.0200793071
C	-2.4357504349	0.7341415023	-0.2053601754
C	-2.6704728612	2.262366838	0.2163281606
C	-3.389141941	0.658918839	-1.5637406846
C	-4.1549646861	2.5070166835	-0.1716640283
C	-1.9793065027	3.1555929959	-0.8684334118
C	-3.9805578214	2.1104669199	-1.6544441939
H	-4.44840193	3.5720907446	-0.0471977317
H	-4.898588181	1.8883187452	0.3648923782
H	-1.8632710299	4.183821178	-0.4686503977
H	-0.9562300652	2.7956539795	-1.0816692004
C	-2.9155827225	3.1243834574	-2.1038529629
H	-4.9054948833	2.1337947847	-2.2680951061
H	-3.3847512673	4.1147712089	-2.28218406
H	-2.4013040559	2.8419975743	-3.0433028257
C	-4.5941269415	-0.3048564401	-1.4450719342
H	-5.193810487	-0.2496646427	-2.3789484316

H	-4.2841418735	-1.3586618149	-1.3136857567
H	-5.2675286151	-0.0583442882	-0.6007744687
C	-2.594099436	0.2489987318	-2.8073452462
H	-2.244453354	-0.7993913489	-2.7313167042
H	-3.2325955149	0.3301798562	-3.7138059032
H	-1.6949989195	0.8694264327	-2.9743178931
C	-2.1609152553	2.6643100536	1.602496714
H	-2.6381077702	2.1301385586	2.4444194
H	-1.0701532717	2.467472473	1.6708121836
H	-2.3102354525	3.7523503951	1.7681122443
C	-2.9436618496	-0.3323726517	0.8083653313
O	-1.0523486377	0.4610834565	-0.3973066182
C	2.0168135308	-3.0000277477	-0.3107007416
C	3.0649388838	-3.0944770789	-1.2556012128
C	2.3425880467	-2.9584560705	1.0648370413
C	4.4036330573	-3.1348890737	-0.8356694681
H	2.8323910182	-3.1008694896	-2.3320081719
C	3.6808418653	-3.0067710548	1.482686826
H	1.5335046972	-2.9023099432	1.8087751736
C	4.7162620765	-3.0928475012	0.5349059946
H	5.2090359474	-3.1918674126	-1.5850469489
H	3.9169727144	-2.9789251445	2.5581162561
H	5.7669567779	-3.1262879788	0.8640829578
Zn	0.0066501505	-0.4282142807	1.1354277147
C	0.0734044358	-0.6497776846	3.1233882205
H	-0.5220122136	-1.5726664303	3.3128960445
H	1.1233477998	-0.9283358292	3.3766964361
Zn	0.4558675408	1.0538907386	-1.6799399752
O	1.6471291903	-0.0320209146	-0.0938464291
C	0.8007062289	0.3755818726	-3.5488276058
H	0.2354169456	1.021236183	-4.2597852287
H	0.3442309668	-0.635880822	-3.6409254823
C	2.5724218794	0.8420034033	-0.3036894161
C	1.6097378093	2.9708290189	-1.2684426597
H	0.9479436074	3.278239647	-2.1167565915
H	2.6338613394	3.0129929119	-1.6916097619
H	3.104334362	0.7853023155	-1.2794665236
C	3.3337303799	1.5092920333	0.7639260078

C	4.5388772251	2.1794093295	0.4373961676
C	2.9130111213	1.4728155728	2.1151585901
C	5.3006905284	2.8030338533	1.4349322908
H	4.8757004065	2.2030563677	-0.6122235888
C	3.6792674874	2.0937699336	3.1115319245
H	1.9833214757	0.9423020887	2.3696959356
C	4.8723466903	2.7623271481	2.7759617207
H	6.2362207974	3.3207670086	1.1697989572
H	3.343798571	2.0570902711	4.1601363976
H	5.4711655788	3.2510444165	3.5611084042
C	-0.4037343744	0.4621263031	4.0693375547
H	-1.4752473118	0.705959586	3.9104810356
H	-0.2972977461	0.1850530207	5.1444521712
H	0.1591658805	1.4116111129	3.9300921964
C	2.2778725687	0.3281187336	-3.9690802055
H	2.767555874	1.3243406892	-3.898074395
H	2.8708649591	-0.3654672664	-3.3322672285
H	2.4205472681	-0.0158509506	-5.0215758493
C	1.4332054261	3.93198253	-0.1008202835
H	2.1445229531	3.7306959699	0.7266006092
H	1.5996519209	4.9942793278	-0.4013870006
H	0.4143604197	3.8872882996	0.3358900358
H	0.4143604197	3.8872882996	0.3358900358

TS 0073

$E(\text{RB-P86}) = -5316.44854150 \text{ A.U.}$

First frequency = $-189.6278 \text{ cm}^{-1}$

C	-2.5883293063	-1.5602433887	0.7689113218
C	-3.8848393953	0.1795501599	1.829448148
C	-4.4049830332	-0.7339018998	2.7592815943
C	-4.0267918398	-2.0808327997	2.7024303448
C	-3.1283122597	-2.4773899815	1.7038364802
C	-1.6392043537	-2.2263377797	-0.1956330832
C	-2.1271197089	-3.0449214226	-1.2326670515
C	-1.2164664715	-3.7974584783	-1.9900787664
C	0.1428035912	-3.7495559925	-1.6665247659
C	0.5747572189	-2.929610217	-0.5971610384

H	-4.2221366914	1.2185942766	1.9046279654
H	-5.1102377527	-0.3814898176	3.5287961037
H	-4.4212819533	-2.8156240551	3.4213989689
H	-2.8183151863	-3.5329473897	1.6397274023
H	-3.2077211182	-3.0936400591	-1.4286048767
H	-1.5714449728	-4.4409940822	-2.8105889514
H	0.8711583882	-4.3731055197	-2.2040834904
N	-0.3151151332	-2.1730524927	0.0963494641
C	-2.4384297145	0.8475945669	-0.2316322826
C	-2.6383132451	2.3881600435	0.1628170732
C	-3.4011055901	0.7631254613	-1.580757272
C	-4.1173489329	2.6608129894	-0.2305877791
C	-1.9287503801	3.2445947046	-0.9379643913
C	-3.9546125487	2.2268804489	-1.7041506738
H	-4.3825311058	3.7358098448	-0.1298945312
H	-4.8783426952	2.0750136347	0.3178721062
H	-1.7935339647	4.27895816	-0.5602756401
H	-0.9132339846	2.8585884995	-1.1403271969
C	-2.8636833751	3.2041463639	-2.1747723347
H	-4.8791130904	2.2612874443	-2.3180977536
H	-3.309124698	4.2004524889	-2.3790395324
H	-2.3542029464	2.8869023683	-3.1057552507
C	-4.6250652421	-0.1714000683	-1.4305655909
H	-5.2911001786	0.1128192154	-0.5923205928
H	-5.2264970563	-0.1338475898	-2.3641928207
H	-4.3333036239	-1.2264422743	-1.2668735921
C	-2.6237305903	0.301539257	-2.8175922279
H	-1.7110443145	0.8953766563	-3.0062975033
H	-2.2985577932	-0.7527220851	-2.7154200289
H	-3.2657955492	0.3739806171	-3.7222459632
C	-2.1194200031	2.8004597914	1.543639975
H	-1.0271733451	2.6102745505	1.6033274081
H	-2.2745688026	3.888476278	1.7047944065
H	-2.585012411	2.2647264825	2.3916352929
C	-2.9627924459	-0.1781416687	0.81603285
O	-1.0656991153	0.5375861834	-0.4339593137
C	1.9987305437	-2.9346866198	-0.167842806
C	2.3330911426	-2.8236697791	1.2013476298

C	3.0410152277	-3.0985333989	-1.1102043165
C	3.6721845789	-2.8751612369	1.6160336497
H	1.531333736	-2.7097747275	1.9461178585
C	4.3807920017	-3.1413448535	-0.6942985903
H	2.8044304126	-3.1573272854	-2.1840809714
C	4.7013786673	-3.0324421921	0.670711584
H	3.9131600256	-2.793748652	2.68763569
H	5.1809796299	-3.2530696488	-1.4430998561
H	5.7528439742	-3.0682917449	0.997074129
Zn	0.0025342568	-0.2781134655	1.1481483834
C	-0.1475874173	-0.0331193956	3.1284849243
H	0.1531319985	1.0055126762	3.3968283323
H	-1.2388311323	-0.0760968412	3.3432223161
Zn	0.4480123405	1.0615882847	-1.7346449427
O	1.6369710482	-0.0029802859	-0.1065814899
C	0.7741729433	0.3100111721	-3.5792004771
H	0.2104962047	0.9363119292	-4.3085269954
H	0.3028906704	-0.6976261762	-3.6297736654
C	2.5829672187	0.8318275468	-0.3721545566
C	1.6445283556	2.95942408	-1.3749422427
H	0.9750110274	3.2699943234	-2.2163033773
H	2.6613762775	2.9707581245	-1.8173744812
H	3.0779126117	0.731040175	-1.3633169857
C	3.4015132731	1.5024019765	0.6497119057
C	4.6102950223	2.1322738394	0.2620151981
C	3.0327067474	1.5060672176	2.0166554087
C	5.4264968365	2.7561307122	1.2152819987
H	4.9063896708	2.1241672017	-0.8000176693
C	3.8532117015	2.1277085502	2.9684637984
H	2.0953703199	1.0145529939	2.3173463459
C	5.0496061932	2.7559415607	2.5723231011
H	6.3643017909	3.2424735041	0.9029806319
H	3.5577113418	2.1240264071	4.0296818835
H	5.6911245209	3.245194032	3.3226439047
C	0.5887006815	-1.0367648616	4.0305903801
H	1.6911035388	-1.0137178383	3.8808135418
H	0.4150667183	-0.8514485322	5.1167223276
H	0.2619819496	-2.0830666703	3.8388798567

C	2.2458675118	0.226639483	-4.0127746858
H	2.8356118968	-0.4556305532	-3.360802661
H	2.3721364869	-0.1527290721	-5.0551281506
H	2.7511944456	1.2169967724	-3.9783879885
C	1.5119133127	3.9432016317	-0.2201850763
H	0.4994535601	3.9316376039	0.233344833
H	2.2311279652	3.7357945647	0.5989571233
H	1.7006311576	4.9961988735	-0.5396790538
H	1.7006311576	4.9961988735	-0.5396790538

TS 0077

E(RB-P86) = -5316.44660371 A.U.

First frequency = -197.7803 cm^{-1}

C	-2.5385639603	-1.6723138995	0.5992745451
C	-3.8269833102	-0.0507044712	1.8450798067
C	-4.3965905433	-1.0626441317	2.6326293221
C	-4.049621395	-2.4004213652	2.4076351129
C	-3.1293849478	-2.6877258665	1.3917910306
C	-1.5752605485	-2.2411992325	-0.4145495429
C	-2.0537056889	-2.9261500687	-1.5488032154
C	-1.1433714346	-3.6401291225	-2.3439817312
C	0.2017094853	-3.6907073538	-1.9656146471
C	0.6243807517	-2.9927633631	-0.8089509456
H	-4.1415130053	0.9790436157	2.0452053405
H	-5.1157789523	-0.7948219866	3.4230038041
H	-4.4836074804	-3.2120555863	3.0121177119
H	-2.8414027533	-3.7340048467	1.200375201
H	-3.127277695	-2.9105924991	-1.7859242487
H	-1.4905062845	-4.1821988053	-3.2378951911
H	0.9222499685	-4.2955742925	-2.5339931981
N	-0.2608849004	-2.2647850073	-0.0803549287
C	-2.3190656832	0.8377328423	-0.0819005555
C	-2.4618429021	2.3180492287	0.5183762385
C	-3.2585291343	0.9795082474	-1.438118723
C	-3.9191934623	2.707954956	0.1460476426
C	-1.6837598609	3.275515008	-0.4432488732
C	-3.7453385373	2.470792926	-1.3692410706

H	-4.1389218066	3.7704917937	0.3882014396
H	-4.7156319742	2.0892090199	0.6001542193
H	-1.5017355737	4.2405366686	0.0737861019
H	-0.6903512558	2.8572136056	-0.681393802
C	-2.6028778377	3.4535750052	-1.6821852384
H	-4.653410378	2.6307349826	-1.9877783286
H	-3.0021050023	4.487641063	-1.7465790261
H	-2.0972183573	3.2515210628	-2.6469411433
C	-4.5186061042	0.0818593646	-1.4267069198
H	-5.1821035407	0.2730340386	-0.5607864401
H	-5.1087387979	0.2699953724	-2.349161491
H	-4.2656549493	-0.9960425687	-1.4081572551
C	-2.4875471877	0.6541983289	-2.7217360649
H	-3.1265887507	0.8487640542	-3.6101624916
H	-1.5659645391	1.2535845718	-2.8483894572
H	-2.1823606335	-0.410541657	-2.749595912
C	-1.9630004117	2.5216291497	1.9498163776
H	-2.0802903576	3.5847208128	2.2495116749
H	-2.4698252656	1.899657295	2.7099292741
H	-0.879956607	2.283902824	2.0066159315
C	-2.8864294136	-0.2997992899	0.815664947
O	-0.9549715614	0.5077991502	-0.3082592022
C	2.0255915487	-3.0999902343	-0.3205216162
C	2.2992183719	-3.0836959245	1.0671133629
C	3.1025030453	-3.2766794431	-1.2211524569
C	3.6117672903	-3.2333633478	1.5387635491
H	1.4687536978	-2.9681509839	1.7791547128
C	4.415921425	-3.4196057231	-0.7477125034
H	2.9167016599	-3.2706122889	-2.3062412893
C	4.6755892592	-3.3993969418	0.6342428224
H	3.8041127147	-3.223044268	2.6232130237
H	5.2436137029	-3.5404002876	-1.4645092813
H	5.7064120875	-3.5135221413	1.0056312631
Zn	0.0917492222	-0.4746757368	1.1828159286
C	0.2107406794	-0.8433271737	3.1445465755
H	-0.1806405893	-1.8826049512	3.2468357557
H	1.2990955708	-0.9130321878	3.3755336331
Zn	0.5361777609	0.8039536414	-1.6806518044

O	1.7150546899	-0.0075714111	-0.0312131505
C	0.8537896414	-0.0630072971	-3.4620203937
H	0.3446778992	0.5370472611	-4.2490195545
H	0.3302757001	-1.0454130832	-3.445692205
C	2.5699618757	0.9572783052	-0.2345017811
C	1.754101322	2.8041386339	-1.4574136486
H	2.8429369509	2.9907036921	-1.4266158379
H	1.313709835	3.3550181003	-0.6005431318
H	3.3049504633	0.7873204777	-1.0525373335
C	3.0769959175	1.8197672241	0.8595983221
C	4.3148199277	2.4885629793	0.6956982706
C	2.3766273359	1.9830576354	2.0770957717
C	4.8352458317	3.2989011056	1.7151900919
H	4.879177593	2.355969928	-0.2426420691
C	2.8966691881	2.7932879583	3.0970648406
H	1.4242365936	1.4511231906	2.2270369867
C	4.1256847337	3.4561005218	2.9201916547
H	5.8021408843	3.8073450164	1.5725903863
H	2.3393562302	2.9061096118	4.0405221461
H	4.5323623863	4.0916588974	3.7229565611
C	-0.477404793	0.0511937441	4.184812694
H	-1.5758274808	0.1003118857	4.0272644278
H	-0.3201482125	-0.3098693791	5.2282571071
H	-0.1062689317	1.0993431322	4.1569501214
C	2.3337480875	-0.2570331019	-3.819368352
H	2.8811129193	0.7097054336	-3.8787044813
H	2.8658988156	-0.8736235436	-3.0624660395
H	2.4824154734	-0.7607473802	-4.804473337
C	1.2283895009	3.3185024899	-2.8101331176
H	0.1229445531	3.2680419427	-2.9097386238
H	1.5065292471	4.3907277961	-2.9551484531
H	1.6548206968	2.7590815474	-3.6685413278
H	1.6548206968	2.7590815474	-3.6685413278

TS 0080

$E(\text{RB-P86}) = -5316.45222365 \text{ A.U.}$

First frequency = $-192.0249 \text{ cm}^{-1}$

C	-2.5694754904	-1.8075218271	0.4056978012
C	-4.0141546768	-0.3305089693	1.6584418627
C	-4.617608381	-1.4159460445	2.3090579841
C	-4.2047764606	-2.7214777305	2.0133330665
C	-3.1929297105	-2.8996527357	1.0628766202
C	-1.5217037441	-2.2832543941	-0.571521112
C	-1.9215167693	-2.9034905797	-1.7721668513
C	-0.9644905778	-3.5979511287	-2.5279379571
C	0.3472613343	-3.6894861913	-2.052654065
C	0.6979379237	-3.0338501204	-0.8484514503
H	-4.3763649758	0.6722920996	1.9101200442
H	-5.4129594715	-1.2323037441	3.0489417409
H	-4.6597568144	-3.5912133987	2.512431329
H	-2.855913013	-3.919117261	0.8153059728
H	-2.9753157358	-2.8610186769	-2.0837059253
H	-1.2507850675	-4.0958735994	-3.4678621292
H	1.095815711	-4.2871655082	-2.59094508
N	-0.2310401094	-2.325446831	-0.1532187535
C	-2.3610605645	0.7631969906	-0.0166358542
C	-2.4599318475	2.1384852533	0.8212840022
C	-3.2591370662	1.1548242245	-1.343602634
C	-3.8544012944	2.7022740083	0.4304632138
C	-1.5548549125	3.1732284345	0.0848303519
C	-3.6014956226	2.6636007644	-1.0909860532
H	-3.9992514227	3.7358707365	0.8135913165
H	-4.7292945447	2.1048908651	0.7490961234
H	-1.4031376264	4.0520512347	0.7455175663
H	-0.5580509223	2.7445831635	-0.117033744
C	-2.3483081249	3.5596495712	-1.1957463547
H	-4.4453577046	3.002787533	-1.7282332145
H	-2.6475085422	4.6286415926	-1.1801961947
H	-1.7774404012	3.4127202921	-2.1347438397
C	-4.5867113253	0.3661390204	-1.4475508153
H	-5.1506510866	0.7129340785	-2.3398086065
H	-4.410398835	-0.7221017534	-1.5649197549
H	-5.2456772653	0.492792094	-0.5673542006
C	-2.5154675457	0.9152965266	-2.6618859997
H	-1.5722743652	1.4890177798	-2.7539450913

H	-2.2638846867	-0.1552004745	-2.7978214656
H	-3.1530170884	1.2246163726	-3.5179349705
C	-2.0739374987	2.0713138079	2.3000747452
H	-1.0292459346	1.710326414	2.4026864343
H	-2.1203959253	3.0847024455	2.7524473739
H	-2.7063821685	1.3998699929	2.9104790812
C	-2.9766740492	-0.4699447954	0.7029359781
O	-1.0102719774	0.4329038788	-0.2955430295
C	2.0659315892	-3.1633492714	-0.2745730536
C	2.2631316002	-3.0947889203	1.1248391203
C	3.1887594667	-3.4124843705	-1.0999908914
C	3.5408876442	-3.2617699714	1.6790085931
H	1.3986947322	-2.9187319136	1.7813510135
C	4.4673196784	-3.574760676	-0.5449333087
H	3.0703339981	-3.4512392813	-2.193499507
C	4.6491408527	-3.50085955	0.8473793277
H	3.6700298424	-3.2087995893	2.7715499
H	5.3293547505	-3.7535798675	-1.2069868856
H	5.6527204408	-3.6297168118	1.2829939727
Zn	0.0733907624	-0.5580582205	1.1577663444
C	-0.1403243939	-0.9563008413	3.1095479746
H	-1.2276218163	-0.8357013891	3.3169619727
H	0.0355133766	-2.0543306464	3.195738138
Zn	0.3952096672	0.6983334849	-1.7635262852
O	1.674671178	-0.0046490785	-0.0546424944
C	0.6583401197	-0.2321807953	-3.5233150873
H	0.3110743983	0.4682864469	-4.3177150951
H	-0.0433029066	-1.0948874582	-3.5601804907
C	2.4307538882	1.0172896292	-0.3195743438
C	1.3848728405	2.712807847	-1.7427838435
H	1.5184471797	3.376811176	-0.8689486693
H	0.3659971584	2.9525797224	-2.1384398014
H	3.123090042	0.9108917236	-1.1846785348
C	2.8902180487	1.9709708089	0.713763774
C	4.0486624912	2.750723026	0.4745412586
C	2.2193861792	2.1142894086	1.9501224207
C	4.5127381046	3.6583836952	1.4377283218
H	4.5936588676	2.6307517724	-0.4757239043

C	2.6853334738	3.0191208216	2.9139235666
H	1.3326512386	1.495533788	2.155569725
C	3.8306923553	3.7978125486	2.6606978196
H	5.4169699771	4.2552209518	1.2381886832
H	2.1533547439	3.1149875204	3.8736653879
H	4.1955983853	4.5079395324	3.4198115944
C	0.6726547362	-0.228109009	4.1892610598
H	0.4442471155	0.8602108332	4.2214884117
H	0.4656122945	-0.6166183945	5.2138833898
H	1.7688741451	-0.3167412414	4.0289500324
C	2.0858323518	-0.7050467102	-3.8307008247
H	2.8060292941	0.1400597228	-3.8837900444
H	2.472332021	-1.391944363	-3.0477826503
H	2.1668292765	-1.2457185602	-4.8041919449
C	2.4155876704	2.9563096961	-2.8365118816
H	2.4683982714	4.0292322341	-3.1364785976
H	3.4467746136	2.6771698883	-2.5241634119
H	2.1902172333	2.3746685564	-3.7544052118
H	2.1902172333	2.3746685564	-3.7544052118

TS 0098

E(RB-P86) = -5316.45367166 A.U.

First frequency = -197.4149 cm⁻¹

C	-2.5615583774	-1.6783232108	0.5768176732
C	-3.9309158249	-0.1032448159	1.7940127144
C	-4.572406077	-1.141490263	2.4841742793
C	-4.2233557811	-2.472358161	2.2207684652
C	-3.2268216854	-2.7223865325	1.270543875
C	-1.5305482871	-2.2257536086	-0.3787431399
C	-1.9440220535	-2.8999763473	-1.5448654757
C	-1.0002805705	-3.644032012	-2.2699821126
C	0.3118352408	-3.7339000316	-1.7947231982
C	0.6747373977	-3.0295570479	-0.6226977836
H	-4.2497955899	0.9209155648	2.0162095178
H	-5.349685856	-0.9011063788	3.2269718354
H	-4.7122201097	-3.306269269	2.7480483584
H	-2.9337316792	-3.7622556937	1.0540892332

H	-2.9979234118	-2.8556929374	-1.8557706786
H	-1.2978590663	-4.1806921816	-3.1847204423
H	1.0510266938	-4.3675426224	-2.3043991392
N	-0.2390687605	-2.2704998883	0.0379493268
C	-2.2892994882	0.8638586144	0.0328530739
C	-2.3480093538	2.2847177365	0.7945737303
C	-3.2148876583	1.1985379963	-1.2941279298
C	-3.7420468427	2.8498506069	0.40307551
C	-1.4435260223	3.2619275538	-0.0169705355
C	-3.5243917903	2.7249117508	-1.1185447288
H	-3.8612564645	3.9047063854	0.7334693509
H	-4.6188710228	2.2853413185	0.7719287727
H	-1.2620689337	4.172533161	0.5911407881
H	-0.4588556946	2.8050136452	-0.2166811863
C	-2.2592145257	3.5915499273	-1.2992192889
H	-4.3765707255	3.0439096959	-1.7551340104
H	-2.5407513238	4.6648064941	-1.3361718331
H	-1.711806725	3.3839237741	-2.240790879
C	-4.5596801658	0.432167162	-1.3238179833
H	-5.1941706482	0.6186371342	-0.4363367306
H	-5.1385559735	0.7434343141	-2.2195803364
H	-4.40785887	-0.664180655	-1.3880264682
C	-2.5088258831	0.8724741192	-2.6139071799
H	-3.1635958536	1.1422447315	-3.4703162554
H	-1.5605658797	1.4256546722	-2.7616498178
H	-2.276039538	-0.2077592223	-2.6937015218
C	-1.9348030379	2.3004631787	2.2677229834
H	-2.0172579845	3.3314688585	2.6731902124
H	-2.5285448186	1.6327777968	2.9200003224
H	-0.87519151	1.9898875252	2.3699906193
C	-2.9149301928	-0.3159738905	0.8281342265
O	-0.952302915	0.4920481264	-0.2635951617
C	2.037708146	-3.1583774409	-0.0392580656
C	2.2198335049	-3.0948861567	1.3622037095
C	3.1671000718	-3.4019854713	-0.8565727175
C	3.4933538341	-3.2600900706	1.9270652092
H	1.3474270833	-2.9304221987	2.0112757697
C	4.4409494331	-3.5619044086	-0.2905554403

H	3.0554393218	-3.4354750699	-1.9511958655
C	4.6093848729	-3.491607587	1.1038513598
H	3.6128522491	-3.2121609166	3.0209176198
H	5.3099622341	-3.7352182425	-0.9448978728
H	5.6094761778	-3.6183143628	1.548034405
Zn	0.1609803096	-0.443424184	1.197358849
C	0.3318240026	-0.5475803633	3.186940478
H	1.4045851523	-0.7570021484	3.4048573377
H	0.1330210811	0.4471330342	3.6448171439
Zn	0.4194371506	0.6572988413	-1.7908262538
O	1.7353248973	-0.0004110786	-0.1154353038
C	0.5985200201	-0.3633982622	-3.5115578017
H	0.249096534	0.309789167	-4.3282783017
H	-0.1298832594	-1.2042872945	-3.4877059344
C	2.5095650876	0.99053614	-0.4362466351
C	1.4501135633	2.649319823	-1.8924150367
H	1.6280667284	3.3456366291	-1.0520849378
H	0.4246278038	2.8979652452	-2.2648160695
H	3.1711872849	0.8404995399	-1.3190650721
C	3.0278831021	1.9651347286	0.5497444481
C	4.1968650226	2.7046233488	0.2429842914
C	2.4087550626	2.1655866351	1.8059155475
C	4.7225880637	3.6275994572	1.1588416926
H	4.7012699935	2.5407916548	-0.7230463121
C	2.9365102172	3.0861957344	2.7219308937
H	1.512174047	1.5817601422	2.0631523765
C	4.0927305388	3.823187206	2.4018531703
H	5.6341035715	4.1924379931	0.9062777212
H	2.4434989299	3.2284348059	3.696693357
H	4.5061447668	4.5453273065	3.123910319
C	-0.5610247975	-1.6018518364	3.8613798614
H	-0.3985261436	-2.6227834023	3.4479170079
H	-0.3884720973	-1.6759941421	4.9608525838
H	-1.6407589944	-1.3825158682	3.7187732863
C	2.0006321616	-0.8955379969	-3.838190827
H	2.0362935738	-1.4780801574	-4.7899723785
H	2.7459138146	-0.0777735662	-3.9460004093
H	2.3870666713	-1.5630440543	-3.0382743378

C	2.4493297193	2.8230592247	-3.0283388642
H	2.5130683418	3.8799353655	-3.3790580056
H	3.4845765331	2.5372148071	-2.7359379705
H	2.1840735271	2.2051660219	-3.9114142217
H	2.1840735271	2.2051660219	-3.9114142217

TS 0114

E(RB-P86) = -5316.45414097 A.U.

First frequency = -194.2861 cm^{-1}

C	-2.5792073971	-1.6707532622	0.6130122482
C	-3.937417576	-0.0357914871	1.762298394
C	-4.6063554444	-1.0409168279	2.4751921423
C	-4.2759454288	-2.3847957662	2.2590863554
C	-3.2727786726	-2.6808204869	1.3292602443
C	-1.5579930286	-2.2642673714	-0.3246280711
C	-1.9927697236	-2.9964642826	-1.4483557713
C	-1.0623516032	-3.7663078803	-2.1628572701
C	0.2662095918	-3.8068362034	-1.7286917907
C	0.651117907	-3.0392830295	-0.6042998689
H	-4.2439100364	0.9995653866	1.9460735039
H	-5.3904425461	-0.764216361	3.1979197882
H	-4.7854589098	-3.1936280288	2.8055022152
H	-2.99638065	-3.7318559369	1.1479103731
H	-3.0547334461	-2.9752793486	-1.7332833729
H	-1.3798987089	-4.3519168556	-3.0401223703
H	1.006757948	-4.4426483331	-2.234111074
N	-0.2562131021	-2.2777624331	0.06050439
C	-2.2536669872	0.8544733489	0.002145034
C	-2.3162788402	2.3008049049	0.7135949735
C	-3.1397541744	1.1512168767	-1.3580884801
C	-3.6945475086	2.8646547528	0.2685347016
C	-1.3818878728	3.2406959489	-0.1092047394
C	-3.4404634352	2.6852800376	-1.2425125665
H	-3.8121595042	3.9314851674	0.5585561656
H	-4.5855530132	2.3208640896	0.6350641224
H	-1.2051974244	4.16968812	0.4718501368
H	-0.3968309108	2.7684349505	-0.2694667802

C	-2.1632899028	3.5346290847	-1.4212460857
H	-4.2739123309	2.9893133423	-1.910443373
H	-2.4340479596	4.6083954211	-1.5000263318
H	-1.595502402	3.2910896373	-2.3416021912
C	-4.488938408	0.3942894406	-1.401341479
H	-5.0416476755	0.6823839031	-2.321083146
H	-4.3439154545	-0.7044352273	-1.4287963289
H	-5.144749636	0.611919051	-0.5367176797
C	-2.3946274654	0.7739018866	-2.6421477632
H	-3.0215376929	1.0116167839	-3.5282244613
H	-1.4408537976	1.3212264422	-2.7798775894
H	-2.1584403391	-0.3085094884	-2.6719054142
C	-1.9361343894	2.3603525097	2.1947633095
H	-2.5680806363	1.7416333318	2.859026126
H	-0.8917693169	2.0138912463	2.3331066064
H	-1.9875567394	3.4087920592	2.5582586327
C	-2.9101193051	-0.2939111319	0.8200947758
O	-0.9142646607	0.4640813501	-0.2490898129
C	2.0453122373	-3.0898486134	-0.089234516
C	2.2946890033	-3.0638089345	1.3023303997
C	3.1413936127	-3.2036420073	-0.9761378097
C	3.6062578331	-3.1501266432	1.7930832191
H	1.4479790122	-2.988840652	2.0011499466
C	4.4527700936	-3.2829416502	-0.4830497658
H	2.9668463563	-3.1918870953	-2.0634301001
C	4.6895704487	-3.2588278177	0.9032198682
H	3.7826351523	-3.1350587725	2.8801568905
H	5.2970913355	-3.3553775618	-1.1869230102
H	5.7191666894	-3.3231713532	1.2897317753
Zn	0.1408791928	-0.4767491126	1.2503810222
C	0.2701757682	-0.5850250933	3.2402946494
H	1.3503461693	-0.7221192878	3.4784221369
H	-0.0049786379	0.3919931249	3.6968728486
Zn	0.5115158595	0.613306975	-1.7288678536
O	1.7609033764	-0.0095091498	0.0152914424
C	0.8747489763	-0.506602976	-3.3584585947
H	0.3668502925	-1.4865319797	-3.2247697343
H	1.9668254756	-0.7276751636	-3.3200059067

C	2.5484943383	0.9756341954	-0.2806914725
C	1.5849695788	2.5823518936	-1.8594489541
H	1.652794622	3.3285121748	-1.0453651617
H	0.6165337235	2.7996064777	-2.3787586686
H	3.265524606	0.8062761233	-1.1155967733
C	2.992204664	1.9812143506	0.711074031
C	4.1962210079	2.6937964154	0.4883895772
C	2.2654146444	2.2346787565	1.8982791084
C	4.6507276826	3.6429143534	1.4160890391
H	4.78762821	2.4853987479	-0.4177511476
C	2.7206075301	3.1816091457	2.8257970079
H	1.3401649204	1.6714276801	2.0915815693
C	3.9126498324	3.8924118368	2.5875167035
H	5.5911985925	4.1854455658	1.2293402328
H	2.142654204	3.3653352327	3.7453762506
H	4.2693653513	4.6354928018	3.3185039225
C	-0.5610585047	-1.7007736753	3.894144041
H	-0.323886052	-2.7062551357	3.478607246
H	-0.4017182519	-1.7702732432	4.996006554
H	-1.6505250506	-1.5525994407	3.7355450799
C	0.5111629282	0.0836843886	-4.7282326335
H	1.0046990751	1.062961145	-4.9140003298
H	0.8033187348	-0.580060532	-5.5766549891
H	-0.5813892703	0.2596286449	-4.8333657991
C	2.7222680539	2.6988176948	-2.8658781935
H	2.7422731009	3.692506536	-3.3720146605
H	3.7209930701	2.5803208617	-2.3922454693
H	2.6531154156	1.9311324474	-3.6651539368
H	2.6531154156	1.9311324474	-3.6651539368

TS 0125

E(RB-P86) = -5316.44819406 A.U.

First frequency = -193.9834 cm⁻¹

C	-2.3886272336	-1.6358358048	0.605793477
C	-3.8589140636	-0.0977191144	1.7522270331
C	-4.4339540701	-1.1423596854	2.4890692364
C	-3.9883346414	-2.4566559093	2.2973863562

C	-2.9792945977	-2.6868809352	1.3553143751
C	-1.3780332319	-2.1796223885	-0.378590391
C	-1.8483141423	-2.8432556791	-1.5295502748
C	-0.963557174	-3.6490577938	-2.2603058924
C	0.3366403864	-3.8306323854	-1.7801902602
C	0.756060627	-3.1430477489	-0.6143956493
H	-4.2433625651	0.9132326483	1.9260949596
H	-5.2317629058	-0.92013033	3.2155191351
H	-4.4182568575	-3.2942061136	2.8684486707
H	-2.6236015057	-3.7152646737	1.1832432833
H	-2.9051173936	-2.7471020664	-1.8182631073
H	-1.2963623732	-4.1566575061	-3.1795210401
H	1.0460304197	-4.4848332444	-2.3063362729
N	-0.0808727604	-2.2780752495	0.0216370168
C	-2.210661188	0.88874753	0.0036095245
C	-2.3178828568	2.3157418084	0.744623842
C	-3.094163963	1.1849007638	-1.3539032746
C	-3.7149277321	2.8399005868	0.3092555109
C	-1.4149477087	3.3045317532	-0.0562356931
C	-3.4527962741	2.7042275891	-1.2047906362
H	-3.8718926662	3.8946740855	0.6234178317
H	-4.5853908799	2.2554512676	0.6619177697
H	-1.2649620409	4.2240865476	0.5465366086
H	-0.4148476728	2.8698166911	-0.2313649971
C	-2.2093643537	3.6051752147	-1.3594984562
H	-4.2960013944	2.9919360141	-1.8675671786
H	-2.5211787717	4.6695965858	-1.4071416154
H	-1.6342949123	3.4109549122	-2.2867497748
C	-4.4138061244	0.3794558604	-1.4205528772
H	-4.9719923131	0.6626047922	-2.3384312014
H	-4.2281871724	-0.7125168894	-1.4652657295
H	-5.0817583502	0.5574489007	-0.556063957
C	-2.3258439045	0.8633289384	-2.6402911563
H	-1.3973064803	1.4563736949	-2.7641952433
H	-2.0413030988	-0.2067430755	-2.6847329009
H	-2.9568183605	1.0872081299	-3.5269537409
C	-1.9493995544	2.3483782372	2.2293625648
H	-1.9945905187	3.3908079253	2.610052854

H	-2.5954869896	1.725229351	2.8755796395
H	-0.909431237	1.9907974953	2.3730117947
C	-2.8208520632	-0.2901998886	0.806450536
O	-0.858083209	0.5350988882	-0.2484804503
C	2.0932767845	-3.4549592976	-0.0267543324
C	2.9408934431	-2.4707303338	0.5289768962
C	2.522734492	-4.8061366168	-0.0091486168
C	4.1803279042	-2.8308118473	1.0828215458
H	2.6481770269	-1.411383609	0.4832981119
C	3.7590239995	-5.1622048275	0.5510476395
H	1.8638527956	-5.593483106	-0.4084717239
C	4.5947382759	-4.1736807075	1.099467021
H	4.8316026733	-2.0470333329	1.5013748487
H	4.0659625866	-6.2201075692	0.5672610693
H	5.565931399	-4.4505994442	1.539726514
Zn	0.2170922399	-0.3881950848	1.2305580044
C	0.4390083299	-0.6327911315	3.195907155
H	1.4879218173	-0.3539187115	3.447004923
H	-0.2038690269	0.0924344857	3.7432172047
Zn	0.5679998583	0.7904332983	-1.7098559252
O	1.8376393468	0.3885842227	0.0740274642
C	1.0627108604	-0.3754139581	-3.2667905787
H	0.7166128854	-1.4075974722	-3.0427290243
H	2.1756747795	-0.4253070986	-3.2465610054
C	2.4782974026	1.4832705257	-0.2158026872
C	1.4555907228	2.8422385698	-1.9615895161
H	1.4852104921	3.6540459166	-1.2114814458
H	0.4705961212	2.9568535376	-2.4801927808
H	3.2638799949	1.4095552286	-0.9999178956
C	2.7038888681	2.5566509299	0.7780386461
C	3.6669157916	3.5639838249	0.5174991378
C	2.0145466837	2.582106784	2.0129998684
C	3.9150522422	4.5772746195	1.4538580347
H	4.2289554114	3.5434252953	-0.4300059343
C	2.2671887516	3.5931661563	2.9514078011
H	1.2902575444	1.7846472469	2.2360823867
C	3.213645855	4.5971940421	2.6744407635
H	4.6665334592	5.3528540537	1.2360722756

H	1.7247963525	3.5943727188	3.9101391657
H	3.4118719254	5.3901855444	3.4130923134
C	0.1493534628	-2.0610660852	3.6851903037
H	-0.9017851166	-2.3614741061	3.4858464673
H	0.7960963471	-2.8116572175	3.1813420522
H	0.3147144527	-2.179850507	4.7818151421
C	0.5819997047	0.0441471101	-4.6624989061
H	0.9050648949	1.0737018729	-4.9336255836
H	0.9650481255	-0.6255851874	-5.4688967038
H	-0.5261644754	0.032155588	-4.7475355585
C	2.5776166214	2.9401383237	-2.9874588162
H	2.5703574233	3.9156488332	-3.5278581407
H	3.5870851225	2.8535596021	-2.5274355592
H	2.5118580923	2.1431029347	-3.7567067045
H	2.5118580923	2.1431029347	-3.7567067045

TS 0127

E(RB-P86) = -5316.45414119 A.U.

First frequency = -194.2774 cm⁻¹

C	-2.544589236	-1.6756898434	0.5257872616
C	-3.9358691438	-0.127629149	1.7531873581
C	-4.5979384991	-1.1808683586	2.3999735024
C	-4.2472762582	-2.5056134246	2.110204552
C	-3.2312706663	-2.734377085	1.1753452263
C	-1.5063829851	-2.200716816	-0.4337801737
C	-1.9202532428	-2.8722994719	-1.6023643633
C	-0.9726081747	-3.5875514811	-2.3501802935
C	0.3520311389	-3.6360804188	-1.9049997703
C	0.7155823288	-2.9298277259	-0.734267208
H	-4.2581801815	0.8913075161	1.9930878001
H	-5.3926354093	-0.9565901607	3.1292514444
H	-4.7510245362	-3.3512105831	2.6037495031
H	-2.9388964472	-3.7695003412	0.9366077625
H	-2.9795651408	-2.8483605219	-1.8967868113
H	-1.2736343338	-4.125562471	-3.2630303872
H	1.105909435	-4.2322705897	-2.4382358491
N	-0.2083544308	-2.2195761418	-0.0364109057

C	-2.2475866642	0.8845537654	0.0646972232
C	-2.337483586	2.2866796594	0.8570576101
C	-3.1241914195	1.2469658081	-1.2857591837
C	-3.7190809254	2.8565364833	0.4303653
C	-1.4083595462	3.2848106813	0.0994715421
C	-3.4475655508	2.7676728967	-1.0856929473
H	-3.8545696007	3.9032682902	0.779745622
H	-4.6059263778	2.2806104775	0.75556878
H	-1.2507288628	4.1812464551	0.7346321027
H	-0.415140235	2.8359759739	-0.0768692797
C	-2.1807103869	3.6429297234	-1.2019177097
H	-4.2785718183	3.0983165466	-1.7439527711
H	-2.4656180203	4.7157322526	-1.2221812344
H	-1.6004743787	3.4600422442	-2.1285416631
C	-4.4621374858	0.4757268921	-1.3867871272
H	-4.3014597135	-0.6175253143	-1.4760023744
H	-5.1293387503	0.6341965793	-0.5180217664
H	-5.0098288148	0.8090238805	-2.2941786334
C	-2.3611492877	0.9541192157	-2.5812841286
H	-2.9822792298	1.2345163059	-3.4589150403
H	-1.4135051093	1.5207242014	-2.6769121526
H	-2.1100729927	-0.1216254066	-2.6708283273
C	-1.9725519647	2.2662412846	2.3431129649
H	-0.9246090404	1.9270756291	2.4721865872
H	-2.0426790022	3.2912274918	2.7655868254
H	-2.6017495739	1.6015755925	2.9641907632
C	-2.8961410549	-0.3175284449	0.8084092011
O	-0.9003683063	0.5272539136	-0.1939148312
C	2.1051596623	-2.9926248556	-0.2081574767
C	2.3405448605	-3.043846313	1.1851407359
C	3.2112832011	-3.0416104519	-1.0885368035
C	3.6482427471	-3.142322926	1.6838789827
H	1.486165221	-3.0197147878	1.8781903892
C	4.5186719766	-3.1331873743	-0.5870692493
H	3.0472859774	-2.9692425422	-2.175128288
C	4.7415392299	-3.1862552223	0.8007013229
H	3.813732839	-3.1878561794	2.771814886
H	5.3707075945	-3.1545359909	-1.2850241333

H	5.7680331485	-3.2602110781	1.1936891003
Zn	0.1522152532	-0.4853598318	1.2598416882
C	0.2629423834	-0.7068528672	3.2414564531
H	1.3426511567	-0.8408613164	3.4833868784
H	-0.0326049018	0.2377344004	3.75051796
Zn	0.5378363832	0.7800058896	-1.6473255914
O	1.7781945634	0.0737219455	0.0715183012
C	0.9326493678	-0.2394122363	-3.3344937222
H	0.4366391859	-1.2318410143	-3.2626791662
H	2.0271485133	-0.4483088978	-3.296879499
C	2.5549259166	1.0847286444	-0.1586279567
C	1.5852772277	2.7672002666	-1.652273601
H	1.6354912019	3.465679655	-0.7957238668
H	0.6188640322	3.0017770019	-2.1677902875
H	3.2825463738	0.9734660365	-0.9941345409
C	2.9747075927	2.0370958363	0.8942227119
C	4.1705032163	2.7778262067	0.7256651293
C	2.2330373636	2.2112940467	2.0864847764
C	4.6025067938	3.6776704156	1.7113978573
H	4.7734553404	2.6304940279	-0.1848434645
C	2.6657624071	3.1089806555	3.0719241691
H	1.3141077302	1.6251662818	2.2372448583
C	3.8497593498	3.8486656108	2.8875754708
H	5.536873514	4.2429631812	1.5661268729
H	2.0764599951	3.2311227677	3.9945371296
H	4.1888124164	4.552913561	3.6639998376
C	-0.5570591624	-1.8712034942	3.8204775941
H	-0.3001590908	-2.847130651	3.3498444058
H	-0.4074439618	-2.0023387001	4.9180828493
H	-1.6471004055	-1.7304461261	3.6591240635
C	0.5750104311	0.4237981497	-4.6720871431
H	0.8841023446	-0.1866337206	-5.5538840993
H	-0.5186313975	0.5919750572	-4.7785952579
H	1.0576543856	1.4181184906	-4.7963591703
C	2.7303343973	2.9564193462	-2.6386690434
H	3.7260556371	2.8245435075	-2.1622582837
H	2.6796631697	2.2348370535	-3.4811124208
H	2.7411498997	3.9776082732	-3.087052764

H 2.7411498997 3.9776082732 -3.087052764