SUPPORTING INFORMATION

The Three Corrugated Surfaces of 1,4-Divinyltetramethylene Diradical Intermediates and their Connections to 1,2-Divinylcyclobutane, 4-Vinylcyclohexene, 1,5-Cyclooctadiene and Two Butadienes

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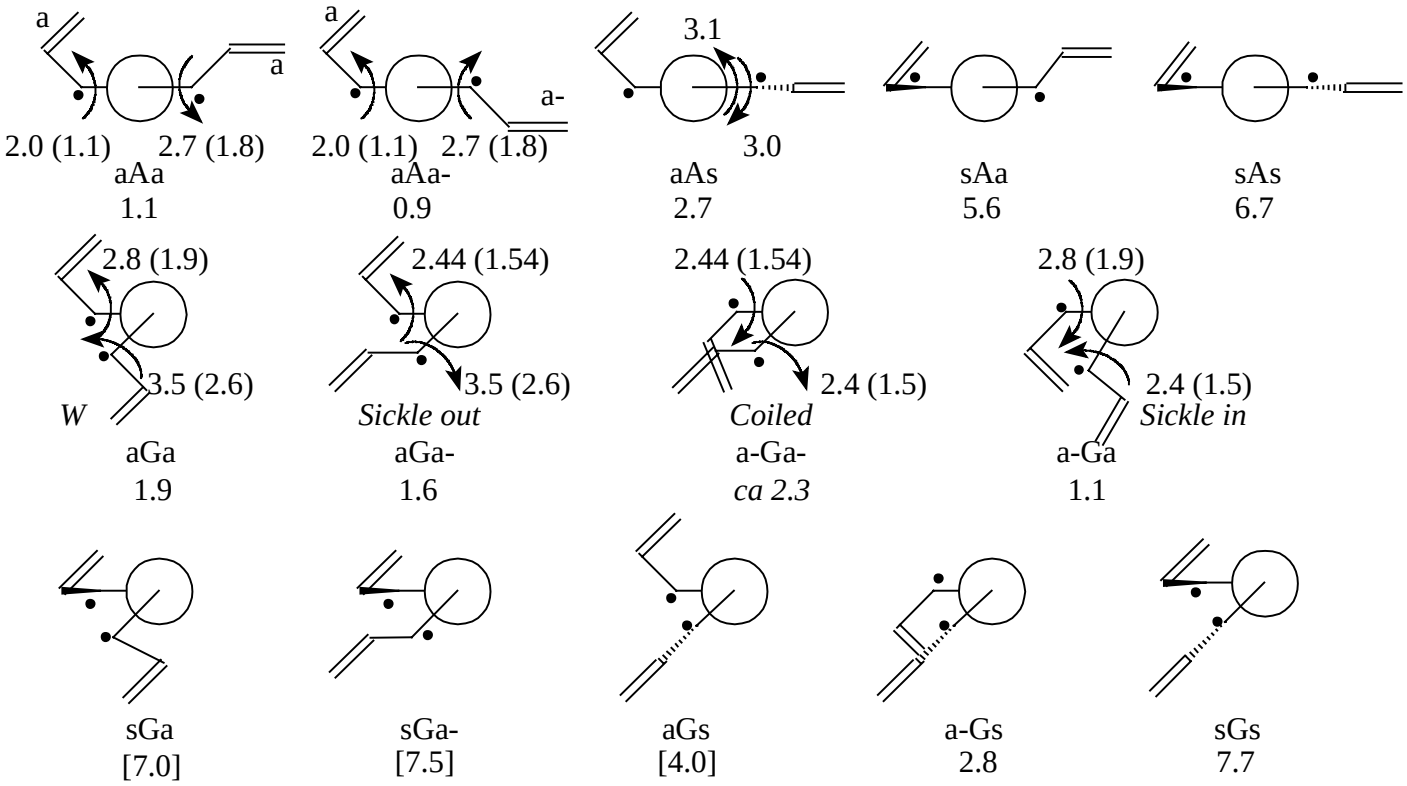
*a) **ct-5** conformers*



*b) **cc-5** conformers*

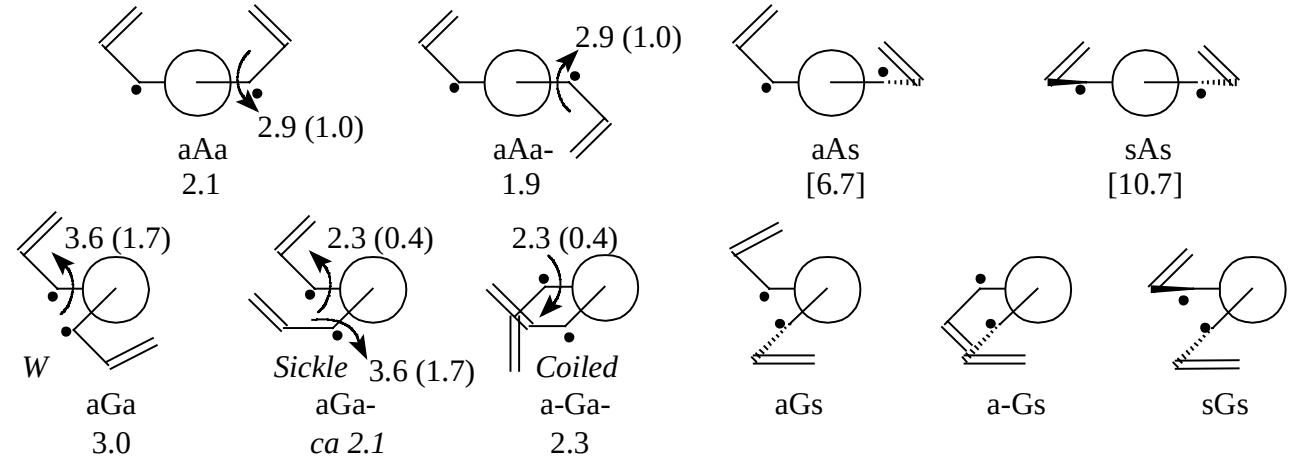


Figure A. The BPW91/6-311+G** conformers of DVT **ct-5** and **cc-5**. Numbers below the symbols and near the arrows specify the energy of the conformers and the rotation TSs, resp., relative to the lowest **tt-5** aAa conformer. Number in parentheses near the arrows indicate the heights of the allylic barriers of the **ct-5** and **cc-5** conformers relative to the lowest **ct-5** aAa- and **cc-5** aAa- conformers, resp. A few **ct** and **cc** high energy conformers involving the synperiplanar allyl moieties are not stable minima, since the steric interference between the two allylic substituents makes the shallow minima of these conformers disappear. In some of these cases the energies of the conformations have been estimated with constrained optimizations and are given in brackets.

Table A. BPW91/6-311+G** electronic energies ΔE_e (kcal/mol), enthalpies, free energies (kcal/mol)[a] and entropies (eu)[a] of the minima and the "allylic" maxima connecting the given minima of the DVT diradicals relative to the lowest[b] **tt-5** aAa conformation.

	Minima				*Maxima*			
Conformers	ΔE_e	ΔH	ΔS	ΔG	ΔE_e	ΔH	ΔS	ΔG
	DVT diradicals ***tt-5***							
aAa	≡0.0[b]	≡0.0	≡0.0	≡0.0	2.0	1.1	-3.0	2.0
aAa-	0.2	0.3	0.6	0.1				
aGa W	0.9	1.0	0.3	0.9	2.7	1.9	-3.0	2.8
aGa- Sickle	0.6	0.6	-0.2	0.6	1.8	1.0	-4.6	2.4
a-Ga- Coiled	1.5	1.3	1.2	1.0				
	DVT diradicals **ct-5**							
aAa	1.1	1.2	1.1	0.9	2.7	1.9	-3.3	2.9
aAa-	0.9	1.1	-0.7	1.3	2.0	1.3	-3.6	2.4
a-Aa-(≡aAa)								
aGa W	1.9	2.0	0.3	1.9	3.5	2.9	-2.9	3.8
aGa- Sickle out	1.6	1.5	1.0	1.3	2.44	1.8	-5.0	3.3
a-Ga- Coiled	(2.1)[c]	(2.1)[c]	(-0.1)[c]	(2.1)[c]	2.4	1.7	-4.5	3.0
a-Ga Sickle in	1.1	1.4	-0.7	1.6	2.8	2.1	-4.2	3.3
(aGa)								
	DVT diradicals **cc-5**							
aAa	2.1	2.4	1.9	1.8	2.9	2.3	-1.1	2.6
aAa-	1.9	2.2	0.9	2.0				
aGa W	3.0	3.3	3.4	2.3	3.6	3.1	-3.4	4.1
aGa- Sickle	[2.1][d]				2.34	1.8	-5.6	3.5
a-Ga- Coiled	2.3	2.3	1.4	1.9				

a. Thermodynamic values at 298.15 K from unscaled vibrational frequencies in the harmonic approximation. b. Electronic energy = –311.986701 hartrees, correction to enthalpy δH = 111.47, S = 98.61. c. BPW91/6-311+G**//6-31G* energy and 6-31G* thermodynamics. d. Estimated values.

Table B. BPW91/6-311+G** electronic energies ΔE_e (kcal/mol), enthalpies, free energies (kcal/mol)[a] and entropies (eu)[a] of the TSs **11** and **12** corresponding to rotation about the central C-C bond of DVT diradicals relative to the lowest **tt-5** aAa conformation.

Isomer	*Barrier*	ΔE_e	ΔH	ΔS	ΔG
			A/G barriers		
tt-5	aA/Ga **11c**	3.6	3.0	-3.5	4.1
	aA/Ga- **11b**	2.8	2.3	-4.5	3.6
	a-A/Ga- **11a**	2.5	2.0	-6.3	3.8
ct-5	aA/Ga	4.2	3.8	-4.9	5.2
	aA/Ga-	3.7	3.2	-4.0	4.4
	a-A/Ga-	3.4	3.0	-4.8	4.4
	a-A/Ga	3.9	3.4	-3.8	4.5
cc-5	aA/Ga	5.1	4.9	-3.2	5.8
	aA/Ga-	4.5	4.3	-5.3	5.8
	a-A/Ga-	4.6	4.3	-3.6	5.4
			G/G- barriers		
tt-5	aG/G-a **12a**	5.2	4.5	-3.6	5.6
	aG/G-a- **12b**	5.7	5.1	-3.5	6.1
ct-5	aG/G-a	5.6	5.1	-3.2	6.0
	aG/G-a-	6.6	6.1	-2.0	6.7
cc-5	aG/G-a	6.9	6.6	-2.7	7.4
	aG/G-a-	[7.8][b]			

a. Thermodynamic values at 298.15 K from unscaled vibrational frequencies in the harmonic approximation. b. Estimated with constrained optimizations.

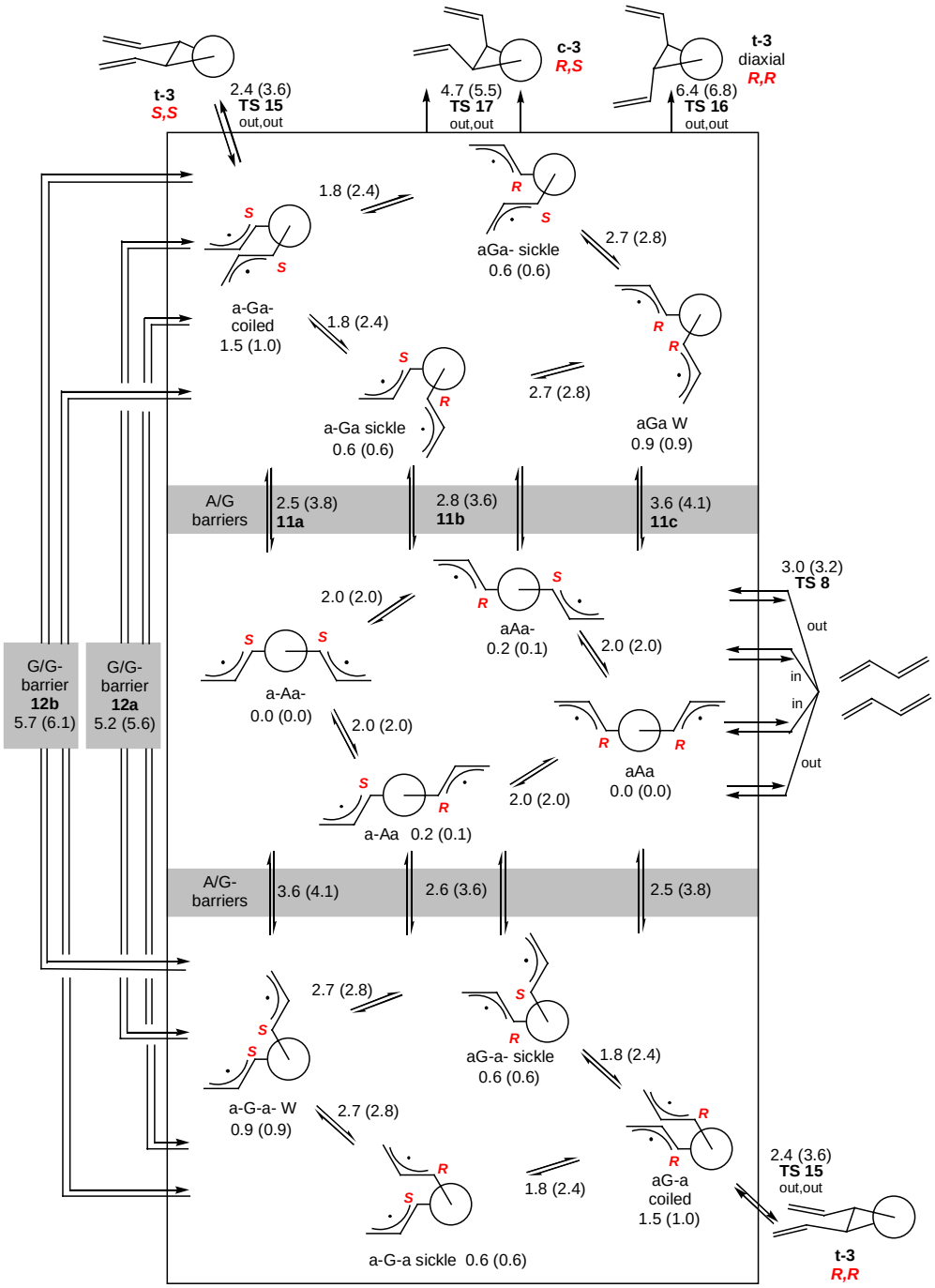


Figure B. Interconversion and connections of the diradicals **tt-5**. Number below the conformational labels and near the arrows specify the electronic energy in kcal/mol of the conformers and the rotation TSs, respectively, relative to the lowest **tt-5** aAa conformer while numbers in parentheses refer to the free energies at 289.15 K. The "allylic" barriers for the interconversions within the G,A and G- families of conformers of diradicals **tt-5** are smaller than the "butane" barriers between the families. The more pertinent free energy barriers between the families are more differenciated than the electronic ones because of the enthalpic and entropic effects given in Table A. Moreover the differences should increase at the experimental temperatures owing to the entropic effects. The heights of the "butane" barriers are comparable to the cyclization TSs of coiled G conformers to tDVCB and to the cleavage TSs of A conformers to butadiene.

Geometries of important structures

Calculattions were performed at the UBPW91/6-311+G(d,p) guess=mix SCF=tight or RBPW91/6-311+G(d,p) SCF=tight level unless otherwise stated with the Gaussian 98 program:

Gaussian 98, Revision A.9; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, Jr., J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M..; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R..; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. Gaussian, Inc., Pittsburgh PA, 1998.

DIRADICALS DVT5

MINIMA

DIRADICAL DVT cc5 aAa E = -311.983277

0 1

C	0.074095	0.522130	0.647111
C	1.488978	0.030656	1.058557
C	0.243025	-0.267517	-0.716277
C	1.782223	-0.244279	-0.441350
H	2.255528	0.621265	-0.928543
H	2.347284	-1.148356	-0.704091
H	-0.145599	-1.289624	-0.585542
H	1.436939	-0.905257	1.633173
H	2.139042	0.736812	1.591718
C	-0.288667	0.337374	-1.971500
H	0.062377	1.353245	-2.194031
H	-1.518256	-1.263897	-2.641405
C	-1.142951	-0.253227	-2.820644
H	-1.495014	0.249727	-3.722745
H	0.114654	1.600625	0.409263
C	-1.137841	0.247987	1.478126
H	-2.092250	0.512109	1.006808
H	-0.230901	-0.558190	3.230491
C	-1.150239	-0.282366	2.709370
H	-2.085534	-0.453015	3.244547

DIRADICAL DVT cc5 aAa- E = -311.983712

0 1

H	1.189436	-0.518001	-3.665708
C	0.481298	-0.138021	-2.921675
H	-1.125505	-0.197311	-4.360077
C	-0.829238	0.034669	-3.337766
H	-1.609337	0.405610	-2.672201
C	1.005908	0.119547	-1.648065
H	2.060109	-0.119264	-1.481560
C	0.232291	0.596586	-0.468284
H	0.848783	1.271129	0.145426
H	-0.659208	1.162930	-0.774929
H	-1.189421	0.517978	3.665725
C	-0.481295	0.137983	2.921689
H	1.125451	0.196957	4.360169
C	0.829203	-0.034895	3.337823
H	1.609291	-0.405860	2.672257
C	-1.005882	-0.119410	1.648034
H	-2.060048	0.119543	1.481508
C	-0.232282	-0.596447	0.468242
H	0.659211	-1.162806	0.774871
H	-0.848789	-1.270976	-0.145470

DIRADICAL DVT cc5 Gcoiled E = -311.983029

0 1

H	1.131649	2.901507	-1.577281
C	0.519458	2.635636	-0.709190
H	-0.404335	4.586064	-0.692888
C	-0.342840	3.604754	-0.223536

H	-0.986808	3.428972	0.638823
C	0.694594	1.342473	-0.200480
H	1.439442	0.702201	-0.680861
C	-0.017932	0.768815	0.989688
H	-1.068663	1.108210	1.010148
H	0.432634	1.152677	1.925636
H	-1.131626	-2.901504	-1.577300
C	-0.519447	-2.635635	-0.709200
H	0.404341	-4.586065	-0.692886
C	0.342841	-3.604756	-0.223534
H	0.986797	-3.428975	0.638834
C	-0.694588	-1.342472	-0.200492
H	-1.439426	-0.702198	-0.680884
C	0.017923	-0.768816	0.989687
H	-0.432656	-1.152681	1.925628
H	1.068654	-1.108211	1.010160

DIRADICAL DVT cc5 Gsickle CONSTRAINED GEOMETRY E = -311.983073

0 1

H	-0.406138	-1.169060	3.377377
C	-0.329672	-0.371119	2.627375
H	-2.240008	0.439209	3.241243
C	-1.384197	0.533914	2.569959
H	-1.405307	1.364592	1.861096
C	0.822209	-0.387240	1.829064
H	1.541234	-1.198219	1.995510
C	1.160592	0.577894	0.736261
H	2.195646	0.941808	0.881946
H	0.507829	1.464981	0.767215
H	-1.914953	-0.615062	-2.458867
C	-0.874476	-0.279483	-2.359245
H	-0.840252	0.343090	-4.430839
C	-0.281334	0.253077	-3.497183
H	0.753919	0.602338	-3.510467
C	-0.298648	-0.442704	-1.091028
H	-0.908531	-0.906855	-0.308934
C	1.091482	-0.050629	-0.696658
H	1.519910	0.666099	-1.418680
H	1.760909	-0.935188	-0.707866

DIRADICAL DVT cc5 Gw E = -311.981985

0 1

H	-2.004539	-3.084626	-0.357252
C	-1.446463	-2.473495	0.360251
H	-1.294907	-4.145984	1.714848
C	-1.055650	-3.098434	1.535852
H	-0.501571	-2.580010	2.318872
C	-1.208694	-1.148169	-0.022510
H	-1.587409	-0.834901	-0.999033
C	-0.462759	-0.125012	0.767187
H	-1.059153	0.800629	0.836143
H	-0.292974	-0.474110	1.796130
H	0.924164	2.617916	-2.461690
C	1.024289	2.303335	-1.417330
H	1.379154	4.340866	-0.802289
C	1.287044	3.301305	-0.490067

```
 H                  1.411706    3.094380    0.573245
 C                  0.867747    0.933665   -1.173597
 H                  0.649416    0.295254   -2.033590
 C                  0.938323    0.268296    0.161096
 H                  1.535679   -0.655262    0.086795
 H                  1.441065    0.918223    0.892559
```

DIRADICAL DVT ct5 aAa E = -311.985021

```
0  1
 H                 -0.165996   -0.584711    3.979981
 C                  0.158117   -0.160873    3.023424
 H                  2.206598   -0.115915    3.697692
 C                  1.513405    0.097955    2.885082
 H                  1.938811    0.517857    1.973199
 C                 -0.852632    0.059317    2.079497
 H                 -1.868937   -0.238025    2.355043
 C                 -0.667742    0.592914    0.700028
 H                 -1.416698    1.376137    0.494433
 H                  0.320497    1.056966    0.576009
 H                  1.220722   -1.003905   -2.162530
 C                  0.486852   -0.302028   -2.576966
 H                  1.607919   -0.092377   -4.416700
 C                  0.727659    0.201905   -3.846568
 H                  0.037565    0.904246   -4.317534
 C                 -0.621007   -0.003759   -1.782084
 H                 -1.362056    0.703286   -2.172397
 C                 -0.834782   -0.525756   -0.403013
 H                 -1.851202   -0.942519   -0.299331
 H                 -0.126442   -1.339085   -0.184263
```

DIRADICAL DVT ct5 aAa- E = -311.985285

```
0  1
 H                 -0.783185   -0.552107    3.935101
 C                 -0.238435   -0.155713    3.071500
 H                  1.640438   -0.312539    4.122333
 C                  1.135005   -0.028135    3.199944
 H                  1.761335    0.364732    2.397930
 C                 -1.009964    0.169599    1.947899
 H                 -2.083307   -0.032644    1.996376
 C                 -0.470318    0.661705    0.649168
 H                 -1.237527    1.237446    0.111442
 H                  0.391880    1.330584    0.799499
 H                 -1.114919   -0.879587   -2.782666
 C                 -0.199378   -0.276864   -2.825773
 H                 -0.356780   -0.042755   -4.971422
 C                  0.205623    0.187190   -4.067100
 H                  1.107610    0.791918   -4.179517
 C                  0.470837   -0.057112   -1.619792
 H                  1.381847    0.552411   -1.640060
 C                 -0.004152   -0.527933   -0.293574
 H                 -0.839959   -1.235084   -0.410967
 H                  0.797254   -1.058794    0.248319
```

DIRADICAL DVT ct5 Gcoiled E = -311.983418 //UBPW91/6-31g(d)

0 1
 H   2.506296   1.274525   1.397213
 C   2.051329   0.578206   0.681046
 H   2.475018   1.916128   -0.966988
 C   2.057549   0.956461   -0.655511
 H   1.647997   0.320722   -1.442948
 C   1.516019   -0.601905   1.213128
 H   1.559687   -0.736912   2.299601
 C   0.785907   -1.645505   0.437615
 H   1.167940   -1.728131   -0.594260
 H   0.938386   -2.629999   0.913113
 H   -2.091018   0.962493   0.846844
 C   -1.916027   0.805911   -0.226407
 H   -2.943999   2.642151   -0.746036
 C   -2.406588   1.761654   -1.103382
 H   -2.271368   1.665167   -2.184555
 C   -1.232714   -0.362139   -0.590379
 H   -1.042321   -0.539918   -1.656959
 C   -0.784267   -1.416699   0.361428
 H   -1.162815   -1.211343   1.377570
 H   -1.211055   -2.390787   0.052175

 DIRADICAL DVT ct5 GsickleIN E = -311.984891

0 1
 C   0.348861   1.177284   -1.789029
 C   1.327798   0.285937   -1.111884
 C   0.215001   0.078664   1.215316
 C   1.425721   0.497815   0.461622
 H   1.640775   1.566450   0.628283
 H   2.302232   -0.068862   0.814277
 H   -0.699140   0.664005   1.079874
 H   1.102188   -0.775089   -1.292848
 H   2.337038   0.475973   -1.509851
 C   0.179156   -1.023440   2.077908
 H   1.110065   -1.592421   2.194003
 H   -1.876396   -0.920931   2.740196
 C   -0.920187   -1.442811   2.807015
 H   -0.864064   -2.302468   3.473756
 H   0.693988   2.178446   -2.061510
 C   -0.994843   0.867137   -2.026997
 H   -1.598331   1.648922   -2.500309
 H   -1.112960   -1.159186   -1.249517
 C   -1.637114   -0.318538   -1.703805
 H   -2.701755   -0.447123   -1.897239

DIRADICAL DVT ct5 GsickleOUT E = -311.984224

0 1
 H   -2.045615   -0.219852   2.717685
 C   -0.969663   -0.059605   2.591268
 H   -0.668508   -0.100585   4.728144
 C   -0.207392   0.013742   3.747745
 H   0.869461   0.183695   3.726203
 C   -0.516118   0.052252   1.271679
 H   -1.258403   -0.004323   0.471004
 C   0.904722   0.258932   0.852138
 H   1.127675   1.341640   0.783704

```
 H                  1.596504   -0.140160    1.610891
 H                 -0.410560   -1.458927   -2.467273
 C                 -0.261196   -0.381839   -2.610153
 H                 -1.504616   -0.366962   -4.382344
 C                 -0.886045    0.212224   -3.698004
 H                 -0.774578    1.278594   -3.902197
 C                  0.545181    0.273492   -1.679601
 H                  0.701494    1.352197   -1.799132
 C                  1.232265   -0.384466   -0.528049
 H                  0.988980   -1.458414   -0.501139
 H                  2.327634   -0.315298   -0.667688
```

DIRADICAL DVT ct5 Gw E = -311.983735

```
0  1
 H                  1.411339   -0.366077   -3.309755
 C                  0.501378   -0.047368   -2.790313
 H                 -0.727277   -0.773297   -4.409190
 C                 -0.702593   -0.285676   -3.435347
 H                 -1.662164    0.004290   -3.005992
 C                  0.685687    0.554327   -1.538847
 H                  1.711317    0.645726   -1.172806
 C                 -0.407040    1.032942   -0.641416
 H                 -0.075208    1.921725   -0.082966
 H                 -1.286750    1.332667   -1.231720
 H                 -0.952483    0.252156    3.138566
 C                 -0.025429   -0.225027    2.797781
 H                  0.723418   -0.392969    4.822137
 C                  0.904145   -0.581007    3.764550
 H                  1.844408   -1.065321    3.494921
 C                  0.114364   -0.427871    1.424307
 H                  1.034816   -0.898847    1.063053
 C                 -0.902341   -0.038239    0.407962
 H                 -1.223694   -0.921909   -0.171919
 H                 -1.797472    0.363705    0.909057
```

DIRADICAL DVT tt5 aAa E = -311.986701

```
0  1
 H                 -1.386671   -0.834704    2.433738
 C                 -0.528383   -0.262668    2.806677
 H                 -1.461726    0.030259    4.737082
 C                 -0.594244    0.218268    4.105721
 H                  0.225644    0.794179    4.538715
 C                  0.546753   -0.094029    1.932154
 H                  1.410139    0.484331    2.280899
 C                  0.577949   -0.588184    0.528538
 H                  1.486303   -1.188217    0.345486
 H                 -0.286140   -1.240066    0.329693
 H                 -1.386672    0.834704   -2.433738
 C                 -0.528383    0.262668   -2.806677
 H                 -1.461726   -0.030259   -4.737083
 C                 -0.594243   -0.218268   -4.105721
 H                  0.225645   -0.794179   -4.538715
 C                  0.546753    0.094029   -1.932154
 H                  1.410139   -0.484331   -2.280899
 C                  0.577949    0.588184   -0.528538
 H                  1.486302    1.188217   -0.345486
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 H                 -0.286141    1.240065   -0.329692


DIRADICAL DVT tt5 aAa-  E = -311.986325

0  1
 H                 -1.457612   -0.188513    2.812224
 C                 -0.374829   -0.100535    2.964742
 H                 -0.630061    0.370806    5.061485
 C                  0.067919    0.220432    4.238827
 H                  1.131951    0.323720    4.459308
 C                  0.440944   -0.339070    1.856676
 H                  1.525430   -0.247035    1.984204
 C                 -0.063415   -0.624597    0.485628
 H                  0.504961   -1.448872    0.026183
 H                 -1.119798   -0.933843    0.517760
 H                  1.457699    0.188719   -2.811936
 C                  0.374959    0.100579   -2.964663
 H                  0.630670   -0.370776   -5.061344
 C                 -0.067493   -0.220483   -4.238827
 H                 -1.131466   -0.323933   -4.459514
 C                 -0.441065    0.339021   -1.856762
 H                 -1.525513    0.246825   -1.984500
 C                  0.062983    0.624653   -0.485622
 H                  1.119326    0.934057   -0.517555
 H                 -0.505606    1.448852   -0.026305


DIRADICAL DVT tt5 Gcoiled  E = -311.984250

0  1
 H                 -0.115522    1.375110   -2.617374
 C                 -0.406297    0.334631   -2.427879
 H                 -2.026900    0.447240   -3.859478
 C                 -1.485236   -0.168033   -3.142159
 H                 -1.828490   -1.194396   -3.001063
 C                  0.338979   -0.369876   -1.483486
 H                  0.063721   -1.410136   -1.275896
 C                  1.530097    0.175378   -0.753819
 H                  2.462944   -0.223322   -1.199994
 H                  1.578983    1.269648   -0.881056
 H                 -0.115527   -1.375112    2.617370
 C                 -0.406298   -0.334631    2.427877
 H                 -2.026902   -0.447239    3.859475
 C                 -1.485236    0.168034    3.142158
 H                 -1.828487    1.194399    3.001065
 C                  0.338981    0.369876    1.483488
 H                  0.063725    1.410137    1.275900
 C                  1.530097   -0.175379    0.753820
 H                  2.462945    0.223320    1.199994
 H                  1.578982   -1.269649    0.881056


DIRADICAL DVT tt5 Gsickle  E = -311.985711

0  1
 H                  0.726874    0.441009   -3.248845
 C                 -0.154418    0.080844   -2.703899
 H                 -1.442614    0.418275   -4.410991
 C                 -1.366822    0.076724   -3.379415
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H	-2.281596	-0.273619	-2.898154
C	0.042680	-0.341559	-1.389112
H	-0.823779	-0.693951	-0.819349
C	1.359295	-0.330384	-0.688783
H	1.677329	-1.362071	-0.447303
H	2.134442	0.088632	-1.350096
H	-0.869858	1.381353	2.018736
C	-0.551137	0.392199	2.368894
H	-2.152612	0.304193	3.823229
C	-1.288093	-0.195209	3.387753
H	-1.021976	-1.175912	3.786312
C	0.567983	-0.166743	1.751465
H	0.899171	-1.158683	2.080823
C	1.351321	0.477676	0.658039
H	0.981894	1.496910	0.466303
H	2.407870	0.572579	0.969692

DIRADICAL DVT tt5 Gw E = -311.985204

0 1

H	1.023033	0.287986	-3.213560
C	0.020592	0.030070	-2.850339
H	-0.876804	0.497823	-4.764192
C	-1.034905	0.155655	-3.742235
H	-2.056865	-0.090427	-3.448291
C	-0.080657	-0.405069	-1.528145
H	-1.073169	-0.666090	-1.146296
C	1.073503	-0.522538	-0.592021
H	1.094967	-1.526703	-0.135100
H	2.017637	-0.396876	-1.145710
H	1.023031	-0.287997	3.213557
C	0.020591	-0.030073	2.850338
H	-0.876805	-0.497830	4.764189
C	-1.034906	-0.155657	3.742234
H	-2.056864	0.090432	3.448291
C	-0.080655	0.405073	1.528146
H	-1.073167	0.666101	1.146299
C	1.073504	0.522539	0.592021
H	1.094971	1.526704	0.135101
H	2.017638	0.396874	1.145711

ALLYL BARRIERS

Allylic barrier DVT cc5 aAa/aAa- E = -311.982076 ν_i = -60

0 1

H	-1.423577	-0.153086	3.760274
C	-0.545488	-0.053910	3.113356
H	0.774376	-0.384973	4.788902
C	0.695532	-0.186060	3.720741
H	1.630058	-0.098011	3.166166
C	-0.806228	0.196441	1.762815
H	-1.853850	0.294191	1.462277
C	0.215296	0.383752	0.682537
H	0.393311	1.466281	0.526674
H	1.186324	-0.037684	0.986818
H	1.412241	0.152930	-3.774618
C	0.542693	0.021217	-3.122115

H	-0.787080	-0.000896	-4.822572
C	-0.696833	-0.066994	-3.738923
H	-1.619478	-0.206303	-3.174918
C	0.807968	-0.044661	-1.750619
H	1.853839	0.014673	-1.435171
C	-0.211209	-0.235643	-0.667257
H	-1.183061	0.185944	-0.972840
H	-0.393493	-1.317904	-0.514209

Allylic barrier DVT cc5 Gcoiled/sickle E = -311.982968 ν_i = -20

0 1

H	0.589279	-2.410640	2.557025
C	-0.209063	-2.057399	1.895844
H	-1.710555	-2.586076	3.352481
C	-1.508242	-2.170259	2.366045
H	-2.370588	-1.853825	1.778543
C	0.199645	-1.541075	0.660519
H	1.270535	-1.551518	0.436792
C	-0.697645	-1.011837	-0.417391
H	-0.950909	-1.824373	-1.125543
H	-1.658218	-0.673668	0.004565
H	0.943366	3.314565	-0.005926
C	0.842169	2.520705	-0.753183
H	1.813881	3.726185	-2.257573
C	1.343235	2.772869	-2.019225
H	1.285550	2.036456	-2.821712
C	0.211064	1.343820	-0.330439
H	-0.140302	1.293097	0.703176
C	-0.044861	0.145195	-1.197401
H	-0.680846	0.425104	-2.058627
H	0.902220	-0.213160	-1.643777

Allylic barrier DVT cc5 Gw/sickle E = -311.980980 ν_i = -41

0 1

H	0.134452	-1.767687	2.990956
C	0.172041	-0.755704	2.573993
H	1.785092	-0.224209	3.906762
C	1.119672	0.105529	3.109774
H	1.236720	1.133371	2.764993
C	-0.744793	-0.476509	1.555666
H	-1.414639	-1.283647	1.249233
C	-0.862708	0.826152	0.819398
H	-1.929598	1.055078	0.652685
H	-0.459371	1.650807	1.425771
H	-0.653386	-1.245373	-3.364172
C	-0.104514	-0.528217	-2.745016
H	1.490295	-0.409192	-4.195878
C	1.107596	-0.067203	-3.234837
H	1.722377	0.645537	-2.684122
C	-0.705409	-0.165540	-1.534638
H	-1.678404	-0.606008	-1.300996
C	-0.142776	0.824065	-0.555264
H	0.931803	0.632245	-0.393773
H	-0.199983	1.843637	-0.985922

Allylic barrier DVT ct5 aAa/aAa- E = -311.982417 ν_i = -58

0 1

H	0.092374	-0.215810	4.202845
C	-0.263515	0.262470	3.284538
H	-1.469894	1.657987	4.406281
C	-1.146220	1.321311	3.421957
H	-1.549048	1.854867	2.560274
C	0.223651	-0.261346	2.081092
H	0.922682	-1.100317	2.138002
C	-0.132089	0.243661	0.714958
H	-1.231790	0.274380	0.595478
H	0.198405	1.294719	0.600633
H	1.219558	-1.569820	-2.883276
C	0.569748	-0.690828	-2.975144
H	0.646963	-0.768396	-5.135093
C	0.260525	-0.258129	-4.253710
H	-0.380417	0.610093	-4.418008
C	0.123579	-0.100849	-1.789212
H	-0.525882	0.777971	-1.861934
C	0.476129	-0.597663	-0.418163
H	0.150101	-1.649532	-0.300462
H	1.576276	-0.624530	-0.296108

Allylic barrier DVT ct5 aAa-/a-Aa- E = -311.983477 ν_i = -43

0 1

H	0.272924	0.208752	4.165270
C	-0.249121	-0.094428	3.251683
H	-1.858396	-0.967882	4.396139
C	-1.454799	-0.762049	3.405344
H	-2.040832	-1.105732	2.552292
C	0.377174	0.231349	2.044080
H	1.342320	0.743425	2.094804
C	-0.150183	-0.097159	0.677664
H	-0.011380	-1.175832	0.469500
H	-1.241102	0.067167	0.639790
H	1.837615	-0.166561	-2.709823
C	0.764007	-0.031413	-2.888670
H	0.951901	-0.654807	-4.954489
C	0.287123	-0.311291	-4.162997
H	-0.769815	-0.196698	-4.409994
C	-0.005251	0.409620	-1.813795
H	-1.081360	0.549240	-1.969047
C	0.530329	0.716720	-0.450358
H	1.617985	0.539617	-0.425294
H	0.384468	1.791227	-0.226852

Allylic barrier DVT ct5 Gcoiled/sickleIN E = -311.982883 ν_i = -58

0 1

H	-1.180324	1.445720	2.953618
C	-0.641306	0.555619	2.612334
H	-1.590936	-0.655484	4.124964
C	-0.886414	-0.626170	3.294497
H	-0.391743	-1.562518	3.034660

C	0.227654	0.740190	1.530662
H	0.325438	1.751927	1.126007
C	1.084800	-0.314912	0.898243
H	0.641856	-1.314643	1.040490
H	2.068447	-0.349479	1.405578
H	0.906852	0.279641	-3.307699
C	-0.028381	0.039338	-2.786949
H	-1.160025	0.120674	-4.628031
C	-1.179279	-0.045465	-3.551579
H	-2.144158	-0.278052	-3.097207
C	0.041366	-0.152207	-1.403516
H	-0.879721	-0.394767	-0.864070
C	1.310295	-0.063056	-0.604022
H	1.772925	0.934818	-0.731648
H	2.058984	-0.777856	-0.994673

Allylic barrier DVT ct5 Gcoiled/sickleOUT E = -311.982809 ν_i = -34

0 1

H	-1.342623	1.468878	-2.556323
C	-0.785835	0.572409	-2.263218
H	-2.209343	-0.686144	-3.287326
C	-1.297386	-0.644971	-2.692947
H	-0.820216	-1.596545	-2.457782
C	0.363324	0.791754	-1.499662
H	0.615139	1.828711	-1.256693
C	1.301474	-0.250295	-0.975934
H	0.950338	-1.262909	-1.224178
H	2.283055	-0.134532	-1.473350
H	0.216768	1.320578	2.469607
C	-0.227885	0.326285	2.341640
H	-1.729263	0.718344	3.852789
C	-1.323908	0.008162	3.133211
H	-1.815188	-0.963369	3.055902
C	0.360335	-0.512282	1.397404
H	-0.071110	-1.508661	1.248480
C	1.549413	-0.157030	0.562167
H	1.901405	0.856209	0.815852
H	2.383845	-0.844749	0.797063

Allylic barrier DVT ct5 Gw/sickleIN E = -311.982283 ν_i = -45

0 1

H	-1.556297	0.826003	-3.255229
C	-0.729510	0.239234	-2.841862
H	-0.503934	-0.853284	-4.690648
C	-0.149135	-0.708147	-3.670827
H	0.675121	-1.341071	-3.340212
C	-0.365975	0.522773	-1.520373
H	-0.933501	1.295989	-0.996769
C	0.745894	-0.155825	-0.774452
H	0.492924	-1.219155	-0.603977
H	1.656216	-0.168854	-1.401588
H	1.086951	-0.775821	3.028218
C	0.126554	-0.286248	2.825193
H	-0.697120	-0.950405	4.714843
C	-0.864693	-0.397088	3.791699
H	-1.843566	0.065923	3.654915

C	0.008842	0.398716	1.616749
H	-0.942741	0.894923	1.398711
C	1.096187	0.494314	0.590851
H	1.345851	1.556331	0.407209
H	2.011105	0.023041	0.982668

Allylic barrier DVT ct5 Gw/sickleOUT E = -311.981058 ν_i = -93

0 1

H	1.465640	-0.129790	-3.117085
C	0.547059	0.201719	-2.621672
H	-0.661447	-0.612572	-4.214886
C	-0.649606	-0.081338	-3.263862
H	-1.615255	0.218138	-2.855241
C	0.708732	0.867211	-1.401595
H	1.729092	1.009114	-1.038086
C	-0.412257	1.369864	-0.537610
H	-0.078824	2.264862	0.012957
H	-1.264626	1.686118	-1.159125
H	-1.060621	-1.586912	2.462818
C	-0.081338	-1.092670	2.452134
H	0.615072	-2.275111	4.124236
C	0.846237	-1.496741	3.398103
H	1.841161	-1.049683	3.442347
C	0.126352	-0.110460	1.480186
H	1.098027	0.392549	1.456291
C	-0.916079	0.318713	0.486500
H	-1.291525	-0.559125	-0.069674
H	-1.796784	0.728877	1.018543

Allylic barrier DVT tt5 aAa/aAa- E = -311.983550 ν_i = -99

0 1

H	1.177296	-0.962132	2.916957
C	0.308229	-0.307231	3.053708
H	0.096954	-0.891206	5.128753
C	-0.283601	-0.281934	4.310019
H	-1.150013	0.349457	4.514896
C	-0.107802	0.430797	1.947163
H	-0.977393	1.088652	2.060179
C	0.552786	0.401964	0.604738
H	0.999504	1.392082	0.386957
H	1.387383	-0.318003	0.612791
H	-1.524013	-0.290059	-3.043588
C	-0.437073	-0.154175	-3.102420
H	-0.457828	-0.342287	-5.257541
C	0.141680	-0.189137	-4.361057
H	1.217672	-0.061399	-4.493298
C	0.246137	0.043329	-1.900355
H	1.332300	0.179188	-1.937941
C	-0.414891	0.057136	-0.550788
H	-1.254090	0.777202	-0.548230
H	-0.880564	-0.925991	-0.345985

Allylic barrier DVT tt5 Gcoiled/sickle E = -311.983810 ν_i = -59

0 1

H	-0.709283	-1.508240	2.457476
C	-0.474974	-0.437243	2.491722
H	-1.919727	-0.094394	4.066751
C	-1.166902	0.339611	3.409947
H	-0.980791	1.411345	3.499403
C	0.495002	0.027134	1.603014
H	0.744095	1.094431	1.617201
C	1.268286	-0.836325	0.653741
H	2.297134	-0.985069	1.035720
H	0.815615	-1.840810	0.604370
H	0.713460	0.978359	-3.148327
C	-0.170545	0.550824	-2.659019
H	-1.464325	1.203614	-4.264839
C	-1.386276	0.688791	-3.307978
H	-2.306443	0.290953	-2.876065
C	0.024625	-0.082029	-1.428227
H	-0.843815	-0.514352	-0.921547
C	1.364087	-0.234991	-0.764198
H	2.029783	-0.865619	-1.385227
H	1.872485	0.745346	-0.704329

Allylic barrier DVT tt5 Gw/sickle E = -311.982392 ν_i = -91

0 1

H	-2.535094	-1.498243	1.819063
C	-1.502834	-1.280093	2.119106
H	-1.991055	-1.480073	4.219806
C	-1.219063	-1.276490	3.478835
H	-0.212877	-1.068034	3.846701
C	-0.586185	-1.032036	1.098908
H	0.448998	-0.810973	1.380286
C	-0.921876	-1.042032	-0.361041
H	-0.355691	-1.845397	-0.870870
H	-1.987959	-1.285828	-0.490278
H	0.616524	2.339885	-2.445018
C	1.346987	1.698648	-1.936456
H	3.002901	2.891254	-2.655293
C	2.686151	2.029619	-2.068976
H	3.466298	1.435630	-1.589220
C	0.846835	0.615979	-1.209634
H	1.563824	-0.034770	-0.698810
C	-0.615917	0.289742	-1.092805
H	-1.147475	1.109231	-0.573174
H	-1.064437	0.246321	-2.102758

BUTANE BARRIERS

Butane A/G Barrier cc5 aA/Ga E = -311.978543 ν_i = -62

0 1

H	-0.875029	-0.033198	3.791247
C	-0.237031	0.048052	2.904933
H	1.449234	-0.757102	3.982470
C	1.076514	-0.367120	3.035919
H	1.787020	-0.318772	2.209729
C	-0.844894	0.562328	1.748964
H	-1.906962	0.813411	1.809420

C	-0.175630	0.719257	0.429444
H	-0.720001	1.443901	-0.189196
H	0.842787	1.116735	0.556416
H	-0.931495	-0.141286	-3.764470
C	-0.256240	-0.115245	-2.902672
H	1.297982	0.798652	-4.086674
C	1.002991	0.421102	-3.108295
H	1.744748	0.485723	-2.311332
C	-0.767683	-0.630024	-1.701271
H	-1.802387	-0.983140	-1.706954
C	-0.045857	-0.655956	-0.401227
H	-0.424846	-1.470613	0.229348
H	1.025934	-0.848675	-0.554768

Butane A/G Barrier cc5 aA/Ga- E = -311.979548 ν_i = -58

0 1

H	1.737123	0.316427	-2.972253
C	0.761040	0.134525	-2.510319
H	0.296381	-1.388266	-3.965169
C	-0.038243	-0.834660	-3.088548
H	-1.026909	-1.080316	-2.698842
C	0.452502	0.916042	-1.384691
H	1.213077	1.617468	-1.033442
C	-0.794941	0.799063	-0.582734
H	-0.938032	1.703362	0.022042
H	-1.676239	0.706240	-1.234832
H	-0.284653	0.294800	3.794405
C	0.032978	-0.026217	2.796646
H	2.079690	-0.188599	3.453501
C	1.379988	-0.297789	2.625634
H	1.792367	-0.626788	1.671440
C	-0.976783	-0.109845	1.826271
H	-1.986162	0.188560	2.124537
C	-0.780175	-0.476736	0.403003
H	0.161519	-1.019084	0.252973
H	-1.586353	-1.150098	0.074062

Butane A/G Barrier cc5 a-A/Ga- E = -311.979283 ν_i = -66

0 1

H	-0.288557	-3.011295	1.635317
C	-0.737188	-2.088679	1.251584
H	-1.528774	-1.621417	3.201416
C	-1.440914	-1.314424	2.159952
H	-1.919822	-0.375685	1.881268
C	-0.533173	-1.833858	-0.110995
H	0.064051	-2.558523	-0.672874
C	-1.019620	-0.651925	-0.874788
H	-1.640580	-0.988805	-1.721226
H	-1.664402	-0.017131	-0.252238
H	0.900159	3.319499	0.054647
C	1.113610	2.278548	-0.211107
H	2.995043	2.360885	0.837669
C	2.313241	1.754275	0.242835
H	2.618112	0.727541	0.039256
C	0.134934	1.633475	-0.978815
H	-0.760102	2.208272	-1.235991

C	0.172686	0.225335	-1.460484
H	0.097734	0.208104	-2.560401
H	1.129571	-0.251169	-1.208534

Butane G/G- Barrier cc5 aG/G-a E = -311.975696 ν_i = -104

0 1

H	-2.233198	-2.106553	-0.785713
C	-1.510600	-1.941384	0.020761
H	-1.321557	-4.067657	0.338008
C	-1.001462	-3.071990	0.642929
H	-0.274829	-3.016095	1.454107
C	-1.205742	-0.605515	0.303560
H	-1.708897	0.163333	-0.287065
C	-0.265435	-0.118185	1.374061
H	-0.788276	0.643703	1.976630
H	-0.011551	-0.931591	2.067225
H	1.029361	1.490819	-2.607239
C	0.973192	1.667338	-1.527672
H	0.749868	3.790175	-1.846833
C	0.808803	2.982541	-1.118139
H	0.735692	3.262246	-0.066713
C	1.073403	0.531764	-0.716481
H	1.202757	-0.433465	-1.211223
C	1.050913	0.514171	0.789101
H	1.914789	-0.073240	1.143176
H	1.187815	1.527435	1.190634

Butane G/G- Barrier cc5 aG/G-a- E = -311.974856 //BPW91/g-31G*constrained

0 1

H	2.985080	0.279766	-1.113434
C	1.999589	-0.158332	-1.318360
H	2.909905	-2.065835	-1.776046
C	1.981947	-1.497138	-1.690109
H	1.056338	-2.036483	-1.904675
C	0.906027	0.705685	-1.169018
H	1.123272	1.740809	-0.886828
C	-0.537185	0.371834	-1.439632
H	-0.908118	1.028527	-2.250519
H	-0.620639	-0.655302	-1.826754
H	-0.188621	0.782252	3.101370
C	-0.707267	0.270028	2.280554
H	-1.101202	-1.433233	3.553364
C	-1.214999	-0.992671	2.560961
H	-1.737056	-1.596486	1.814951
C	-0.774054	0.973170	1.069750
H	-0.328367	1.972832	1.048884
C	-1.475065	0.522719	-0.183771
H	-2.279094	1.247512	-0.418568
H	-1.985449	-0.436123	-0.003993

Butane A/G Barrier ct5 aA/Ga E = -311.979976 ν_i = -56

0 1

H	-0.821850	-0.675058	3.857211
C	-0.284779	-0.213869	3.021736

H	1.576741	-0.282405	4.110494
C	1.072740	-0.000906	3.186503
H	1.686842	0.458410	2.411054
C	-1.050384	0.098523	1.888220
H	-2.111200	-0.162669	1.910955
C	-0.513700	0.689817	0.631338
H	-1.340368	1.043296	0.001595
H	0.109006	1.571662	0.849856
H	1.310249	0.767761	-2.600241
C	0.423932	0.140143	-2.754531
H	0.417290	0.533176	-4.881801
C	-0.062534	0.024609	-4.046538
H	-0.937406	-0.588960	-4.269231
C	-0.109701	-0.489403	-1.626208
H	-1.000113	-1.114567	-1.757976
C	0.398985	-0.309867	-0.242974
H	0.438830	-1.271688	0.288078
H	1.424629	0.086759	-0.265268

Butane A/G Barrier ct5 a-A/Ga E = -311.980541 ν_i = -67

0 1

H	0.032384	-0.645443	3.874666
C	0.267308	-0.183414	2.909768
H	2.365728	-0.139441	3.402743
C	1.602023	0.096312	2.662584
H	1.941978	0.553966	1.733170
C	-0.825909	0.056226	2.065909
H	-1.810169	-0.267278	2.418364
C	-0.772074	0.645355	0.703481
H	-1.478878	1.487570	0.630876
H	0.221597	1.058459	0.486543
H	-0.911367	0.794948	-2.924125
C	-0.050755	0.156442	-2.689456
H	0.915554	0.636451	-4.564218
C	0.967988	0.086114	-3.625622
H	1.850932	-0.532913	-3.456305
C	-0.087481	-0.532828	-1.473596
H	0.763784	-1.171225	-1.213615
C	-1.168653	-0.387616	-0.461763
H	-2.095079	-0.036402	-0.939269
H	-1.391144	-1.358241	0.003341

Butane A/G Barrier ct5 aA/Ga- E = -311.980803 ν_i = -68

0 1

H	1.715498	-0.239143	-3.317749
C	0.744612	-0.084430	-2.835105
H	-0.273685	-1.043718	-4.476795
C	-0.371153	-0.548444	-3.511446
H	-1.380866	-0.440140	-3.113635
C	0.772391	0.564955	-1.592082
H	1.751293	0.830844	-1.184214
C	-0.414059	0.840548	-0.735591
H	-0.259953	1.769616	-0.169643
H	-1.314931	0.986411	-1.347739
H	0.999079	-1.203264	2.295513
C	0.308141	-0.430932	2.654430

H	1.149530	-0.491048	4.646526
C	0.412027	-0.043859	3.981234
H	-0.246737	0.717636	4.402678
C	-0.611910	0.072059	1.731135
H	-1.303561	0.853889	2.066046
C	-0.695197	-0.343823	0.308582
H	0.000443	-1.171748	0.109777
H	-1.705227	-0.725783	0.082291

Butane A/G Barrier ct5 a-A/Ga- E = -311.981232 ν_i = -61

0 1

H	1.011776	-1.028055	3.262036
C	0.762356	-0.334731	2.451677
H	2.832331	0.227299	2.236292
C	1.811091	0.369600	1.884644
H	1.664773	1.075644	1.067000
C	-0.592876	-0.265205	2.098129
H	-1.283811	-0.935970	2.616923
C	-1.164682	0.571147	1.010234
H	-2.124982	1.000294	1.332773
H	-0.505395	1.416286	0.771527
H	0.527040	-1.457053	-1.865988
C	0.297053	-0.441226	-2.208459
H	1.734327	-0.569475	-3.818806
C	0.990476	0.039541	-3.306678
H	0.808203	1.042186	-3.697852
C	-0.689027	0.255581	-1.503123
H	-0.921641	1.279408	-1.818709
C	-1.426652	-0.273550	-0.329086
H	-2.512825	-0.252890	-0.517209
H	-1.156220	-1.324612	-0.152018

Butane G/G- Barrier ct5 aG/G-a E = -311.976946 ν_i = -114

0 1

H	1.866037	-0.037621	-2.555047
C	0.791026	0.039163	-2.359413
H	0.351541	-1.115675	-4.129880
C	-0.052890	-0.585546	-3.268447
H	-1.138112	-0.574007	-3.163326
C	0.429601	0.757274	-1.215957
H	1.236519	1.170131	-0.605154
C	-0.969268	1.029106	-0.744390
H	-1.089713	2.121604	-0.640676
H	-1.698095	0.717023	-1.504168
H	-0.117435	0.656937	3.091809
C	0.283255	-0.201825	2.539103
H	1.635679	-0.708213	4.153756
C	1.270265	-0.958080	3.158475
H	1.710416	-1.826562	2.665352
C	-0.245430	-0.441612	1.271983
H	0.139669	-1.291746	0.699922
C	-1.338436	0.368637	0.641737
H	-2.215226	-0.284615	0.479894
H	-1.667787	1.147701	1.345386

Butane G/G- Barrier ct5 aG/G-a- E = -311.976209 ν_i = -123

0 1

H	0.144199	-1.256607	2.839137
C	-0.318401	-1.464180	1.868289
H	-2.169257	-2.011890	2.831415
C	-1.638189	-1.890912	1.888007
H	-2.194633	-2.118827	0.978488
C	0.498091	-1.265096	0.749933
H	1.526596	-0.948080	0.936017
C	0.118527	-1.521971	-0.681106
H	0.739084	-2.351091	-1.067381
H	-0.919016	-1.876962	-0.738037
H	-1.001778	2.141442	-1.312850
C	0.000174	2.159133	-0.867241
H	-0.217746	4.227682	-0.268126
C	0.421862	3.346135	-0.286027
H	1.406685	3.432054	0.176726
C	0.741286	0.978800	-0.931817
H	1.748878	0.983397	-0.505147
C	0.279508	-0.273245	-1.622045
H	0.990923	-0.521215	-2.430493
H	-0.682662	-0.074098	-2.117329

Butane A/G Barrier tt5 a-A/Ga- 11a E = -311.982686 ν_i = -55

0 1

H	-1.061960	-1.176791	1.829630
C	-0.620507	-0.291326	2.302326
H	-2.265040	-0.116673	3.696157
C	-1.316652	0.291326	3.348866
H	-0.931598	1.173095	3.864429
C	0.608928	0.146230	1.801366
H	1.059112	1.040069	2.248390
C	1.321099	-0.468591	0.653274
H	2.373043	-0.664526	0.915179
H	0.869233	-1.437505	0.396917
H	-1.061960	1.176791	-1.829630
C	-0.620507	0.291326	-2.302326
H	-2.265040	0.116673	-3.696157
C	-1.316652	-0.291326	-3.348866
H	-0.931598	-1.173095	-3.864429
C	0.608928	-0.146230	-1.801366
H	1.059112	-1.040069	-2.248390
C	1.321099	0.468591	-0.653274
H	2.373043	0.664526	-0.915179
H	0.869233	1.437505	-0.396917

Butane A/G Barrier tt5 aA/Ga- 11b E = -311.982165 ν_i = -64

0 1

H	1.064093	0.451096	-3.179888
C	0.069803	0.059293	-2.932554
H	-0.690424	0.525726	-4.903876
C	-0.903670	0.115040	-3.917794
H	-1.912552	-0.261187	-3.738929
C	-0.099511	-0.471275	-1.651222
H	-1.086323	-0.861440	-1.378363

C	0.949692	-0.474241	-0.596128
H	0.982458	-1.451413	-0.091953
H	1.940238	-0.310109	-1.045034
H	-1.415251	0.805135	2.277913
C	-0.571219	0.247394	2.701386
H	-1.630456	-0.104316	4.555080
C	-0.715531	-0.257994	3.984327
H	0.086453	-0.821150	4.465054
C	0.565237	0.117143	1.899957
H	1.415545	-0.447777	2.299560
C	0.690973	0.648089	0.518371
H	-0.207183	1.223664	0.249441
H	1.538759	1.351069	0.452935

Butane A/G Barrier tt5 aA/Ga 11c E = -311.980886 ν_i = -60

0 1

H	-1.399840	-0.059865	2.964089
C	-0.303074	-0.069096	2.981895
H	-0.254845	0.441510	5.084332
C	0.320206	0.220131	4.186091
H	1.408215	0.225253	4.273525
C	0.345766	-0.388752	1.786812
H	1.441517	-0.397883	1.781842
C	-0.349246	-0.636057	0.494114
H	0.119777	-1.474393	-0.040804
H	-1.396748	-0.919193	0.674970
H	-1.399840	0.059866	-2.964088
C	-0.303074	0.069096	-2.981895
H	-0.254846	-0.441511	-5.084332
C	0.320206	-0.220132	-4.186090
H	1.408214	-0.225256	-4.273525
C	0.345767	0.388752	-1.786812
H	1.441518	0.397881	-1.781843
C	-0.349244	0.636059	-0.494114
H	0.119781	1.474394	0.040804
H	-1.396745	0.919197	-0.674970

Butane G/G- Barrier tt5 aG/G-a 12a E = -311.978393 ν_i = -121

0 1

H	0.416803	-0.924390	2.985328
C	-0.262035	-0.199519	2.519301
H	-1.783034	-0.541144	4.023440
C	-1.497092	0.001242	3.123130
H	-2.219514	0.708866	2.712581
C	0.191548	0.443327	1.369159
H	-0.471588	1.166630	0.883269
C	1.541474	0.231370	0.756109
H	2.107002	1.179800	0.808909
H	2.106961	-0.491326	1.363101
H	0.416806	0.924386	-2.985330
C	-0.262034	0.199518	-2.519301
H	-1.783031	0.541141	-4.023443
C	-1.497092	-0.001242	-3.123132
H	-2.219514	-0.708863	-2.712581
C	0.191546	-0.443325	-1.369158
H	-0.471591	-1.166627	-0.883266

C	1.541474	-0.231371	-0.756108
H	2.107000	-1.179802	-0.808908
H	2.106961	0.491324	-1.363101

Butane G/G- Barrier tt5 aG/G-a- 12b E = -311.977578 ν_i = -119

0 1

H	-0.422359	-1.335758	2.477754
C	-0.466118	-0.255004	2.295946
H	-2.154887	-0.020717	3.630351
C	-1.449784	0.466346	2.957984
H	-1.551402	1.544291	2.820084
C	0.473816	0.276062	1.413193
H	0.452029	1.354709	1.229939
C	1.561540	-0.521591	0.753773
H	2.542630	-0.142488	1.094105
H	1.503230	-1.563081	1.104003
H	-0.513753	-1.302880	-2.481533
C	-0.553057	-0.225274	-2.280983
H	-2.291783	0.025398	-3.546454
C	-1.562631	0.503717	-2.893743
H	-1.661320	1.579000	-2.734699
C	0.418406	0.294280	-1.425926
H	0.402191	1.369915	-1.225283
C	1.531002	-0.511368	-0.819701
H	1.459225	-1.548290	-1.180838
H	2.498222	-0.127453	-1.192867

THERMOLYSIS of DVCB 3

CIS DVCB c-3 inin E = -312.025882

0 1

C	0.286818	0.817761	-0.794546
C	1.464762	-0.139985	-1.137892
C	1.388828	-0.726391	0.298521
C	0.620966	0.545952	0.743898
H	0.435055	1.870687	-1.086628
H	2.393958	0.423695	-1.301461
H	1.331814	-0.833873	-1.977451
H	2.331495	-0.953845	0.814241
H	0.743567	-1.615476	0.327888
H	1.345726	1.321111	1.048497
C	-1.092782	0.399280	-1.215547
C	-1.424551	-0.580323	-2.067243
H	-1.902154	0.986197	-0.766090
H	-2.468694	-0.786278	-2.307422
H	-0.679847	-1.208485	-2.559375
C	-0.475056	0.497285	1.760901
C	-0.853501	-0.577316	2.466507
H	-0.992340	1.448374	1.938232
H	-1.657930	-0.519814	3.201311
H	-0.373552	-1.549873	2.340671

CIS DVCB c-3 inout E = -312.027581

0 1

C	0.145688	0.826943	-0.660935
C	1.438657	0.178524	-1.236027
C	1.517123	-0.733268	0.016587
C	0.550225	0.237763	0.767291
H	0.136015	1.929522	-0.661720
H	2.262863	0.904639	-1.271180
H	1.374211	-0.311016	-2.216192
H	2.500559	-0.902418	0.475776
H	1.039074	-1.707537	-0.159484
H	1.128264	1.003431	1.307397
C	-1.176684	0.351873	-1.188804
C	-1.398396	-0.441289	-2.246237
H	-2.043816	0.723021	-0.629399
H	-2.412871	-0.708993	-2.545568
H	-0.588695	-0.845850	-2.856402
C	-0.491831	-0.338238	1.667269
C	-0.702050	0.029738	2.940035
H	-1.112811	-1.130987	1.234191
H	-1.473256	-0.439842	3.553001
H	-0.105930	0.813750	3.414506

CIS DVCB c-3 outin E = -312.027995

0 1

C	0.333951	0.657264	-0.738470
C	1.461501	-0.398462	-0.899232
C	0.439026	0.493910	0.841282
C	1.833791	-0.182257	0.592711
H	2.057373	-1.073639	1.193966
H	2.652776	0.539760	0.718486
H	0.730813	1.659167	-0.978882
H	0.470097	1.442902	1.396073
H	2.234917	-0.201044	-1.653518
H	1.054660	-1.404783	-1.074957
C	-0.577695	-0.416087	1.454639
H	-0.713245	-1.390508	0.971227
H	-1.217163	0.834030	3.052678
C	-1.312460	-0.125588	2.537957
H	-2.032507	-0.835069	2.948825
C	-0.993329	0.496358	-1.411140
H	-1.773376	1.190136	-1.075886
H	-0.551921	-1.107514	-2.742048
C	-1.289665	-0.394499	-2.367667
H	-2.283147	-0.437265	-2.816449

CIS DVCB c-3 outout E = -312.028285

0 1

C	0.240223	0.565507	-0.786676
C	1.748236	0.174586	-0.973877
C	1.718714	-0.524639	0.410368
C	0.442432	0.301975	0.770205
H	-0.020522	1.605705	-1.029880
H	2.392230	1.065265	-0.974896

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 H                  1.994645   -0.436523   -1.852648
 H                  2.588108   -0.410991    1.071923
 H                  1.488369   -1.596682    0.322923
 H                  0.743622    1.254320    1.233968
 C                 -0.705471   -0.364172   -1.480946
 C                 -1.751898    0.018792   -2.226460
 H                 -0.502596   -1.437046   -1.376279
 H                 -2.399245   -0.707131   -2.720998
 H                 -1.996344    1.074542   -2.367426
 C                 -0.641239   -0.328667    1.580420
 C                 -1.140917    0.171776    2.719951
 H                 -1.041610   -1.276008    1.202051
 H                 -1.928545   -0.340786    3.274710
 H                 -0.778599    1.114396    3.138638


TRANS DVCB 3 inin  E = -312.030021

0  1
 C                 -0.029335   -0.474979   -0.635801
 C                  1.499748   -0.223641   -0.744300
 C                 -0.029335    0.474979    0.635801
 C                  1.499748    0.223641    0.744300
 H                  1.719299   -0.621013    1.413150
 H                  2.133831    1.074261    1.026479
 H                 -0.209417    1.502310    0.273003
 H                  1.719299    0.621013   -1.413150
 H                  2.133831   -1.074261   -1.026479
 C                 -0.964574    0.176620    1.763648
 H                 -2.030859    0.271322    1.524148
 H                  0.426872   -0.283776    3.310581
 C                 -0.617470   -0.184657    3.007253
 H                 -1.369942   -0.386402    3.771027
 H                 -0.209417   -1.502310   -0.273003
 C                 -0.964574   -0.176620   -1.763648
 H                 -2.030859   -0.271322   -1.524148
 H                  0.426872    0.283775   -3.310581
 C                 -0.617470    0.184657   -3.007253
 H                 -1.369942    0.386401   -3.771027


TRANS DVCB 3 inout  E = -312.031525

0  1
 C                  0.074095    0.522130    0.647111
 C                  1.488978    0.030656    1.058557
 C                  0.243025   -0.267517   -0.716277
 C                  1.782223   -0.244279   -0.441350
 H                  2.255528    0.621265   -0.928543
 H                  2.347284   -1.148356   -0.704091
 H                 -0.145599   -1.289624   -0.585542
 H                  1.436939   -0.905257    1.633173
 H                  2.139042    0.736812    1.591718
 C                 -0.288667    0.337374   -1.971500
 H                  0.062377    1.353245   -2.194031
 H                 -1.518256   -1.263897   -2.641405
 C                 -1.142951   -0.253227   -2.820644
 H                 -1.495014    0.249727   -3.722745
 H                  0.114654    1.600625    0.409263
 C                 -1.137841    0.247987    1.478126
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H	-2.092250	0.512109	1.006808
H	-0.230901	-0.558190	3.230491
C	-1.150239	-0.282366	2.709370
H	-2.085534	-0.453015	3.244547

TRANS DVCB 3 outout E = -312.032068

0 1

C	0.279378	-0.260780	-0.748147
C	1.817048	0.016650	-0.775183
C	0.279372	0.260786	0.748154
C	1.817047	-0.016614	0.775192
H	2.029319	-1.025310	1.160107
H	2.446707	0.703249	1.315010
H	0.096762	1.347656	0.746305
H	2.029301	1.025351	-1.160097
H	2.446722	-0.703200	-1.315000
C	-0.609230	-0.409974	1.741030
H	-0.481703	-1.495871	1.834977
H	-1.691611	1.281618	2.441473
C	-1.528739	0.202602	2.501056
H	-2.150312	-0.350024	3.207438
H	0.096790	-1.347653	-0.746299
C	-0.609234	0.409963	-1.741025
H	-0.481743	1.495866	-1.834957
H	-1.691545	-1.281657	-2.441508
C	-1.528709	-0.202635	-2.501075
H	-2.150290	0.349978	-3.207460

Opening tDVCB TS15inin E = -311.981790 ν_i = -151

0 1

H	-1.763242	1.003801	2.319617
C	-0.822100	0.449741	2.238629
H	-1.185341	-0.547004	4.111112
C	-0.514158	-0.421553	3.261975
H	0.404667	-1.008989	3.270200
C	-0.049621	0.710090	1.090253
H	-0.383439	1.512681	0.427938
C	1.286714	0.097334	0.762177
H	1.392582	-0.881561	1.256525
H	2.131605	0.718278	1.114123
H	-1.763725	-1.003126	-2.319446
C	-0.822329	-0.449481	-2.238579
H	-1.184986	0.546866	-4.111392
C	-0.513920	0.421355	-3.262170
H	0.405200	1.008332	-3.270528
C	-0.050016	-0.709838	-1.090090
H	-0.384202	-1.512109	-0.427578
C	1.286587	-0.097586	-0.762165
H	2.131217	-0.718818	-1.114230
H	1.392726	0.881276	-1.256518

Opening tDVCB TS15inout E = -311.982174 ν_i = -186

0 1

C	0.103601	0.741170	1.124826

C	1.362652	-0.073014	0.966398
C	0.287626	-0.416322	-1.184406
C	1.622220	-0.125759	-0.546907
H	1.997466	0.849203	-0.900056
H	2.390605	-0.874173	-0.819044
H	-0.282801	-1.252981	-0.768678
H	1.209018	-1.095209	1.346017
H	2.212884	0.347489	1.535321
C	-0.180073	0.183347	-2.367013
H	0.430287	0.992390	-2.786305
H	-1.992833	-0.948164	-2.664829
C	-1.340882	-0.152536	-3.030181
H	-1.649918	0.370178	-3.934834
H	0.062020	1.672559	0.554787
C	-0.935683	0.493036	2.041508
H	-1.771026	1.200982	2.022659
H	-0.217613	-1.285404	3.050936
C	-1.007082	-0.539694	2.952987
H	-1.862358	-0.638236	3.620754

Opening tDVCB TS15outout E = -311.982792 ν_i = -212

0 1

C	0.358400	-0.374223	-1.239953
C	1.706865	0.103171	-0.761171
C	0.358400	0.374223	1.239953
C	1.706865	-0.103171	0.761171
H	1.825241	-1.173845	0.995831
H	2.543174	0.421625	1.261152
H	0.056482	1.379437	0.928767
H	1.825241	1.173845	-0.995831
H	2.543174	-0.421625	-1.261152
C	-0.445168	-0.297512	2.175350
H	-0.101125	-1.285436	2.504868
H	-2.031890	1.147352	2.408607
C	-1.632806	0.173017	2.696415
H	-2.215629	-0.416190	3.403639
H	0.056482	-1.379437	-0.928767
C	-0.445168	0.297512	-2.175350
H	-0.101125	1.285436	-2.504868
H	-2.031890	-1.147352	-2.408607
C	-1.632806	-0.173017	-2.696415
H	-2.215629	0.416190	-3.403640

Opening tDVCB diaxial TS16inin E = -311.976372 ν_i = -241

0 1

H	2.462310	-1.831331	0.405781
C	2.186195	-0.793662	0.189757
H	3.930933	-0.528133	-1.046031
C	3.028606	-0.075971	-0.635572
H	2.836911	0.965330	-0.897879
C	1.004598	-0.329047	0.795422
H	0.505687	-0.989543	1.505806
C	0.441121	1.071830	0.635572
H	1.235259	1.834447	0.583563
H	-0.170757	1.310331	1.517736
H	-2.462310	-1.831331	-0.405781

C	-2.186195	-0.793662	-0.189757
H	-3.930933	-0.528133	1.046031
C	-3.028606	-0.075971	0.635572
H	-2.836911	0.965330	0.897879
C	-1.004598	-0.329047	-0.795422
H	-0.505687	-0.989543	-1.505806
C	-0.441121	1.071830	-0.635572
H	0.170757	1.310331	-1.517736
H	-1.235259	1.834447	-0.583563

Opening tDVCB diaxial TS16inout E = -311.976454 ν_i = -281

0 1

C	-0.294471	0.886318	0.944412
C	1.199092	0.698971	0.738659
C	0.155313	-0.639577	-1.046402
C	1.372024	-0.560423	-0.138260
H	2.312352	-0.537204	-0.714677
H	1.407611	-1.458826	0.494539
H	-0.619746	-1.370246	-0.803243
H	1.747434	0.622300	1.692599
H	1.598486	1.579973	0.213150
C	0.050480	0.061617	-2.260689
H	0.875105	0.738125	-2.517740
H	-1.846040	-0.690516	-2.963789
C	-0.994780	-0.034323	-3.155003
H	-1.004339	0.538453	-4.081756
H	-0.795649	1.638636	0.334341
C	-1.046927	0.258502	1.954107
H	-2.116190	0.494824	1.975470
H	0.478112	-0.892728	2.978008
C	-0.573519	-0.609387	2.917406
H	-1.240414	-1.032977	3.667711

Opening tDVCB diaxial TS16outout E = -311.976446 ν_i = -312

0 1

C	0.171294	0.638864	1.095642
C	1.574531	0.576955	0.511802
C	0.171288	-0.638857	-1.095635
C	1.574528	-0.576958	-0.511799
H	2.343893	-0.445482	-1.292099
H	1.794425	-1.528878	-0.005137
H	-0.489082	-1.442962	-0.762765
H	2.343899	0.445473	1.292104
H	1.794435	1.528874	0.005141
C	-0.263197	0.177648	-2.154722
H	0.441852	0.933051	-2.523830
H	-2.243994	-0.624253	-2.452157
C	-1.496437	0.106052	-2.767716
H	-1.764200	0.773427	-3.586198
H	-0.489064	1.442986	0.762789
C	-0.263203	-0.177655	2.154715
H	0.441836	-0.933075	2.523808
H	-2.243985	0.624274	2.452166
C	-1.496439	-0.106051	2.767712
H	-1.764210	-0.773431	3.586185

Opening cDVCB TS17inin E = -311.979451 ν_i = -129

0 1

H	0.137577	1.510620	2.731851
C	0.175281	0.562025	2.185768
H	1.919725	-0.059591	3.285231
C	1.193765	-0.312533	2.513073
H	1.313491	-1.277946	2.021549
C	-0.818758	0.368101	1.213919
H	1.353491	1.596879	-1.983480
C	0.818359	0.657988	-1.807550
H	2.566463	-0.499103	-2.307975
C	1.520611	-0.515730	-2.002985
H	1.057177	-1.496395	-1.888693
C	-0.521663	0.772831	-1.404022
C	-1.406987	-0.400613	-1.044759
H	-1.326262	-1.221558	-1.777279
H	-2.460111	-0.079538	-1.044443
C	-0.997789	-0.865048	0.368197
H	-1.731754	-1.565290	0.812330
H	-0.046786	-1.413744	0.300181
H	-0.966612	1.769299	-1.402997
H	-1.593322	1.134251	1.123872

Opening cDVCB TS17inout E = -311.979374 ν_i = -246

0 1

H	2.365139	-1.443953	-0.482681
C	1.356263	-1.340990	-0.895654
H	1.033849	-3.467848	-0.799189
C	0.622933	-2.495709	-1.069780
H	-0.379792	-2.487166	-1.498628
C	0.941387	-0.030955	-1.202637
H	1.689445	0.761369	-1.148734
C	-0.432110	0.322772	-1.738686
H	-0.387050	1.295899	-2.252186
H	-0.799349	-0.409030	-2.476934
H	-1.069294	-0.223762	2.178359
C	-0.541139	0.703922	1.929016
H	0.055788	1.013298	3.978768
C	0.080376	1.383657	2.954425
H	0.625452	2.311820	2.771778
C	-0.541009	1.089044	0.577351
H	-0.053339	2.033314	0.313856
C	-1.347565	0.414137	-0.504403
H	-2.299517	0.942168	-0.709711
H	-1.616149	-0.601371	-0.172490

Opening cDVCB TS17outin E = -311.978588 ν_i = -223

0 1

H	-0.515982	-1.449757	-1.509011
C	-0.523132	-0.392665	-1.800327
H	-2.409261	-0.614153	-2.821999
C	-1.594693	0.052904	-2.542000
H	-1.663139	1.091664	-2.871049
C	0.565455	0.395465	-1.385095

H	0.596170	1.436813	-1.716987
C	1.773984	-0.169868	-0.663452
H	2.574630	0.585156	-0.644452
H	2.187269	-1.057166	-1.173836
H	-1.190121	1.561451	2.208608
C	-0.713339	0.604896	1.969701
H	-2.233532	-0.477616	3.042694
C	-1.322401	-0.537018	2.448164
H	-0.921088	-1.533553	2.261231
C	0.459771	0.676732	1.198236
H	0.864885	1.670900	0.992373
C	1.321985	-0.487361	0.773659
H	2.170771	-0.655370	1.464722
H	0.733624	-1.416875	0.774393

Opening cDVCB TS17outout E = -311.979167 ν_i = -263

0 1

H	-0.251638	-1.388812	1.946260
C	-0.595314	-0.350267	1.865172
H	-2.514230	-0.840571	2.720077
C	-1.868128	-0.065383	2.309468
H	-2.271284	0.947947	2.261083
C	0.303564	0.580141	1.314192
H	-0.001090	1.629741	1.289160
C	1.728188	0.233911	0.919965
H	2.317048	1.159388	0.826662
H	2.232296	-0.387211	1.680002
H	-0.498029	-1.486144	-1.888316
C	-0.437624	-0.394513	-1.971054
H	-2.136105	-0.322235	-3.300428
C	-1.366110	0.238391	-2.771519
H	-1.364960	1.323227	-2.893731
C	0.568354	0.241906	-1.227814
H	0.674855	1.326964	-1.330958
C	1.642690	-0.474905	-0.443837
H	2.613386	-0.492171	-0.977245
H	1.346030	-1.525807	-0.299997

TS18 Cope cDVCB E = -311.995671 ν_i = -389

0 1

H	-1.716107	1.513499	1.186836
C	-1.452652	0.571271	0.694728
H	-1.450578	-0.483279	2.570356
C	-1.210484	-0.526364	1.507469
H	-1.117907	-1.527659	1.088477
C	-1.079083	0.656953	-0.656178
H	1.721497	1.511643	1.180478
C	1.455431	0.570262	0.688151
H	1.461653	-0.487399	2.562083
C	1.216260	-0.528383	1.500335
H	1.120392	-1.528793	1.079935
C	1.076267	0.658111	-0.661072
C	0.770045	-0.559675	-1.538064
H	1.203846	-1.481630	-1.123699
H	1.193910	-0.434878	-2.545284
C	-0.775899	-0.562309	-1.532030

H	-1.208590	-0.442705	-2.536141
H	-1.202811	-1.484321	-1.110810
H	1.324227	1.584837	-1.185189
H	-1.329348	1.582637	-1.181043

CONNECTIONS TO VCH AND COD

COD 4 twist-boat E = -312.056794

0 1

C	-0.883623	-0.118530	1.567951
C	1.063700	1.406016	-0.776964
C	-0.620349	1.128126	1.136628
C	-0.384231	1.618681	-0.276019
H	1.748372	1.971052	-0.119471
H	-0.586884	2.700995	-0.304427
H	-1.094799	1.169193	-0.981010
C	-0.549165	-1.450547	-0.663004
H	-0.763613	-2.457788	-1.053674
C	-1.037345	-1.410379	0.804667
H	-2.101883	-1.711699	0.832556
H	-0.507651	-2.196535	1.371785
H	-1.012592	-0.236462	2.650131
H	-0.540379	1.898873	1.910894
C	0.932878	-1.184533	-0.823022
C	1.583126	-0.007594	-0.865236
H	-1.148374	-0.765234	-1.275700
H	1.169604	1.882840	-1.770066
H	1.556814	-2.082345	-0.890649
H	2.671547	-0.062956	-0.983247

COD 4 chair E = -312.053155

0 1

C	-0.125135	-0.888590	-1.639288
C	0.273293	0.384374	-1.808409
C	-0.273290	-0.384376	1.808408
C	0.942166	1.269018	-0.779821
C	0.125139	0.888588	1.639287
C	-0.006660	1.720200	0.382567
H	1.813670	0.755382	-0.340194
H	1.333335	2.163101	-1.287197
H	0.209729	2.769308	0.632210
H	-1.046052	1.696487	0.014124
C	0.006661	-1.720201	-0.382567
H	1.046052	-1.696491	-0.014123
H	-0.209730	-2.769309	-0.632210
C	-0.942165	-1.269017	0.779820
H	-1.813667	-0.755378	0.340193
H	-1.333337	-2.163099	1.287196
H	-0.621694	-1.374601	-2.485462
H	0.073352	0.847100	-2.780358
H	-0.073347	-0.847103	2.780356
H	0.621700	1.374599	2.485460

TS21cN toVCH E = -311.981442 ν_i = -39

0 1

H	-1.505960	-1.284042	2.546438
C	-0.744730	-0.536898	2.297926
H	-1.551309	0.822109	3.768251
C	-0.788699	0.655466	3.008421
H	-0.077032	1.464108	2.840633
C	0.161096	-0.900835	1.298412
H	0.041297	-1.890745	0.847824
C	1.295036	-0.075033	0.775388
H	2.251085	-0.554173	1.059659
H	1.305240	0.923696	1.237083
H	-1.505759	1.284247	-2.546483
C	-0.744649	0.536993	-2.297937
H	-1.551479	-0.821970	-3.768164
C	-0.788829	-0.655408	-3.008356
H	-0.077298	-1.464161	-2.840527
C	0.161253	0.900842	-1.298460
H	0.041618	1.890798	-0.847926
C	1.295066	0.074886	-0.775402
H	2.251186	0.553894	-1.059653
H	1.305142	-0.923846	-1.237092

TS21tN toVCH E = -311.983497//ubpw91/6-31G(d) ν_i = -28

0 1

H	2.931049	-0.966781	-0.243338
C	2.004410	-0.564985	-0.672752
H	1.263138	-2.554280	-1.102908
C	1.088552	-1.478970	-1.178955
H	0.174886	-1.165808	-1.686182
C	1.838995	0.824314	-0.636773
H	2.629233	1.426917	-0.176589
C	0.587223	1.527111	-1.029149
H	0.802646	2.586546	-1.245722
H	0.141089	1.098245	-1.943552
H	-0.746156	-0.132731	2.308572
C	-1.363095	-0.492558	1.473761
H	-2.193959	-2.093622	2.669619
C	-2.171488	-1.591988	1.700218
H	-2.816511	-1.997355	0.915124
C	-1.280817	0.232883	0.272265
H	-1.890506	-0.103596	-0.576418
C	-0.533039	1.507294	0.105400
H	-1.245063	2.305613	-0.182143
H	-0.074290	1.818244	1.059445

TS21tX to VCH E = -311.984857 ν_i = -34

0 1

C	-0.484045	-0.145447	-2.158592
C	-1.264241	0.586474	-1.134418
C	-0.340196	-0.521106	1.046913
C	-1.533800	-0.254451	0.208376
H	-2.019849	-1.192397	-0.099312
H	-2.270585	0.326864	0.785245
H	0.322200	-1.343401	0.765067
H	-0.771006	1.521864	-0.831317

H	-2.256059	0.851349	-1.529322
C	-0.039472	0.212571	2.207882
H	-0.733399	1.020255	2.472916
H	1.759376	-0.794716	2.849631
C	1.030570	-0.007399	3.050660
H	1.178659	0.593356	3.947335
H	-1.040759	-0.711269	-2.909882
C	0.908777	-0.270533	-2.141330
H	1.356853	-0.919008	-2.901413
H	1.409531	1.027265	-0.471773
C	1.761589	0.319274	-1.220675
H	2.829944	0.103537	-1.230072

TS23 to COD E = -311.973663 ν_i = -202

0 1

H	1.628392	0.237151	-2.572393
C	1.137159	-0.231257	-1.712848
H	3.007871	-0.302036	-0.619011
C	1.939118	-0.513283	-0.601320
H	1.554147	-1.047978	0.264452
C	-0.228977	-0.451333	-1.828055
H	-0.707163	-0.161874	-2.767991
C	-1.132214	-1.036653	-0.769718
H	-1.981769	-1.524695	-1.272076
H	-0.606165	-1.828132	-0.210714
H	0.512903	0.537090	2.961952
C	0.137634	0.692278	1.944787
H	1.779247	2.033807	1.490518
C	0.885845	1.535372	1.115592
H	0.547724	1.808903	0.118327
C	-1.016378	0.000697	1.601305
H	-1.473747	-0.627352	2.370915
C	-1.698092	0.012857	0.254602
H	-2.768747	-0.193512	0.407603
H	-1.637259	1.016557	-0.197647

CONNECTIONS TO BUTADIENE AND CYCLOADDITIONS TSs

butadiene-trans E = -156.008708

0 1

C	1.758260	0.000000	0.600664
H	2.331165	0.000000	1.528202
H	2.328725	0.000000	-0.331030
C	0.410852	0.000000	0.600664
C	-0.410852	0.000000	-0.600664
H	-0.124017	0.000000	1.556564
C	-1.758260	0.000000	-0.600664
H	0.124017	0.000000	-1.556564
H	-2.328725	0.000000	0.331030
H	-2.331165	0.000000	-1.528202

VCH2 E = -312.066894

0 1

C	-0.000024	-0.148328	-0.593076
C	1.247052	-0.034134	1.622615
C	-1.258256	-0.169807	1.623452
C	0.095109	-0.214851	2.288208
C	-1.191982	0.427561	0.207538
C	1.323736	0.194912	0.132758
H	-1.683894	-1.190148	1.586579
H	0.119264	-0.402024	3.365866
H	-1.076724	1.523104	0.277053
H	1.597160	1.248703	-0.066805
H	2.194573	-0.057046	2.169461
H	-1.957799	0.414026	2.245272
H	-2.132494	0.240281	-0.332453
H	2.143528	-0.404057	-0.297214
H	-0.101636	-1.248075	-0.609908
C	0.009958	0.350215	-2.013783
H	0.081273	1.439324	-2.131878
H	-0.130097	-1.506098	-3.041744
C	-0.059695	-0.417268	-3.109615
H	-0.048533	0.012205	-4.112808

VCH COPE TS22 E = -311.995186 ν_i = -353

0 1

C	1.408676	0.581321	0.553247
C	1.408675	-0.581322	-0.553250
H	1.841973	-0.136812	-1.464864
C	0.066319	-1.148957	-0.897223
H	-0.057794	-2.230197	-0.960611
C	-0.897267	-0.288204	-1.429000
H	1.841975	0.136810	1.464860
H	2.100119	1.373158	0.233729
C	0.066321	1.148957	0.897222
C	-0.897264	0.288205	1.429002
H	-0.057791	2.230197	0.960611
H	-1.895881	0.683293	1.635332
C	-0.702676	-1.088289	1.407646
H	-1.529153	-1.767979	1.625028
H	0.290417	-1.522729	1.512106
H	2.100118	-1.373159	-0.233733
C	-0.702677	1.088290	-1.407644
H	-1.895884	-0.683291	-1.635329
H	0.290416	1.522729	-1.512106
H	-1.529154	1.767980	-1.625025

TS7CN E = -311.983684 ν_i = -377

0 1

C	0.321829	-0.156778	1.145918
C	-0.125314	1.785500	0.739245
H	-0.907131	1.815250	1.500194
C	-0.516045	1.956672	-0.595998
H	0.193849	2.365801	-1.316742
C	-1.794370	1.534990	-1.079193
H	1.360703	-0.031680	0.835750
H	0.185489	-0.138229	2.229169
C	-0.474739	-1.036630	0.400202
C	-0.272098	-1.255084	-0.998362

H	-1.323484	-1.529517	0.877289
H	-0.976621	-1.924476	-1.500096
C	0.663999	-0.616509	-1.758623
H	0.717780	-0.777626	-2.835627
H	1.426840	0.030118	-1.326638
H	0.812027	2.244760	1.059878
C	-2.737847	0.894740	-0.329607
H	-1.986073	1.668458	-2.147654
H	-2.639439	0.762751	0.747289
H	-3.664249	0.536774	-0.779522

TS7CX E = -311.982982 ν_i = -392

0 1

C	1.079132	0.644492	-0.024806
C	0.700990	-0.533238	1.584545
H	1.133263	-1.465870	1.222440
C	-0.661549	-0.528487	1.912900
C	-1.322568	0.508224	2.678071
H	-1.272477	-1.381505	1.616540
H	0.511555	1.478152	0.399033
H	2.162079	0.765257	0.056042
C	0.583400	-0.019295	-1.151390
C	-0.804829	-0.225018	-1.374981
H	1.285512	-0.571404	-1.781686
H	-1.084472	-0.916845	-2.175417
C	-1.798238	0.284155	-0.578633
H	-2.839555	-0.001298	-0.734339
H	-1.618211	1.077511	0.143552
H	1.379682	0.049215	2.212618
C	-0.780951	1.663944	3.139002
H	-2.384142	0.333062	2.881454
H	0.269069	1.922729	2.990140
H	-1.381892	2.380263	3.698951

TS7TN E = -311.981533 ν_i = -421

0 1

C	-1.305950	-3.258055	1.823874
C	-1.202297	-1.348989	1.011299
H	-0.691852	-1.641998	0.091889
C	-0.575117	-0.390934	1.825455
H	-2.005476	-2.913809	2.587270
H	-1.781889	-3.810350	1.010461
C	-0.007556	-3.605960	2.202734
C	0.687850	-2.883554	3.202408
H	0.565866	-4.283907	1.565369
H	1.761278	-3.064287	3.307276
C	0.128031	-1.838645	3.900209
H	0.736860	-1.209203	4.549236
H	-0.949336	-1.714962	3.989500
H	-2.289034	-1.301918	0.921393
H	-1.188084	0.185443	2.523505
C	0.753769	0.120967	1.543895
C	1.263486	1.288622	1.996172
H	1.362496	-0.486195	0.863893
H	2.259960	1.622709	1.707608
H	0.695381	1.942824	2.661518

TS7TX E = -311.983667 ν_i = -408

0 1

C	-1.354715	-3.132593	1.942613
C	-1.193994	-1.417850	0.924387
H	-0.548555	-1.778322	0.123522
C	-0.731576	-0.339736	1.704886
C	-1.633899	0.523610	2.431201
H	0.318147	-0.047830	1.649962
H	-1.952317	-2.690251	2.742122
H	-1.944408	-3.740756	1.251994
C	-0.049032	-3.559050	2.230093
C	0.806028	-2.840004	3.102661
H	0.402736	-4.322189	1.590953
H	1.864907	-3.115890	3.109437
C	0.416693	-1.726384	3.805576
H	1.145327	-1.118694	4.343573
H	-0.627845	-1.475025	3.971467
H	-2.254760	-1.402562	0.655383
C	-1.299090	1.664017	3.082029
H	-2.690973	0.229304	2.419878
H	-0.265518	2.013954	3.127137
H	-2.051815	2.277697	3.576503

TS 8ccIN E = -311.977754 ν_i = -235

0 1

H	-0.072488	0.310622	-3.677238
C	0.173936	0.067868	-2.638445
H	2.177568	0.783158	-2.892940
C	1.444961	0.343056	-2.216879
H	1.790660	0.114769	-1.207831
C	-0.885393	-0.487794	-1.860429
H	-1.863213	-0.554023	-2.345080
C	-0.814987	-0.783898	-0.474143
H	-1.674060	-1.329374	-0.076448
H	0.130380	-1.190298	-0.090767
H	-0.072494	-0.310640	3.677235
C	0.173934	-0.067874	2.638445
H	2.177566	-0.783169	2.892935
C	1.444960	-0.343057	2.216879
H	1.790659	-0.114759	1.207834
C	-0.885389	0.487799	1.860429
H	-1.863210	0.554035	2.345078
C	-0.814977	0.783902	0.474144
H	-1.674042	1.329385	0.076444
H	0.130396	1.190288	0.090768

TS 8ccOUT E = -311.976755 ν_i = -764

0 1

H	-3.837229	0.137306	0.192368
C	-2.861901	-0.245541	0.510270
H	-3.713746	-2.148121	0.998977
C	-2.812781	-1.537091	0.952882
H	-1.884634	-2.010242	1.277575

C	-1.771962	0.672039	0.396653
H	-1.982792	1.614238	-0.117596
C	-0.422752	0.398505	0.733329
H	0.225399	1.269611	0.864959
H	-0.259229	-0.360664	1.502726
H	3.837248	-0.137243	-0.192399
C	2.861904	0.245568	-0.510295
H	3.713695	2.148145	-0.999111
C	2.812744	1.537097	-0.952965
H	1.884578	2.010214	-1.277653
C	1.771988	-0.672030	-0.396606
H	1.982850	-1.614199	0.117684
C	0.422764	-0.398543	-0.733266
H	0.259204	0.360605	-1.502675
H	-0.225362	-1.269673	-0.864869

TS 8ctIN E = -311.979441 ν_i = -732

0 1

H	-0.049622	0.334859	-3.920093
C	0.209384	0.037000	-2.898784
H	2.286969	0.414345	-3.264739
C	1.530800	0.094141	-2.548581
H	1.886114	-0.182631	-1.554843
C	-0.884798	-0.354558	-2.072164
H	-1.885706	-0.212323	-2.489035
C	-0.789973	-0.725719	-0.700866
H	-1.674255	-1.218906	-0.290180
H	0.131103	-1.229758	-0.395041
H	1.489767	0.153021	1.837788
C	0.548882	0.069569	2.395292
H	1.555216	-0.612557	4.166226
C	0.606823	-0.367216	3.689157
H	-0.296199	-0.470475	4.294288
C	-0.634014	0.459429	1.711101
H	-1.579987	0.373655	2.256442
C	-0.677152	0.800086	0.330719
H	-1.566116	1.350507	0.013872
H	0.243006	1.223872	-0.089933

TS 8ctOUT E = -311.979894 ν_i = -729

0 1

H	-0.720474	-0.650000	3.871615
C	-0.232748	-0.160930	3.022071
H	1.654128	-0.161378	4.039111
C	1.105479	0.101165	3.135065
H	1.675868	0.589359	2.343231
C	-1.067651	0.112805	1.898934
H	-2.083143	-0.291161	1.933838
C	-0.626157	0.681162	0.671121
H	-1.418829	1.012117	-0.003735
H	0.181997	1.415379	0.738195
H	-1.066870	-0.934762	-2.696302
C	-0.184457	-0.287971	-2.772368
H	-0.513392	0.076941	-4.863478
C	0.101948	0.272161	-3.985771
H	0.967822	0.923795	-4.119747

C	0.586795	-0.124498	-1.589921
H	1.459121	0.535974	-1.649790
C	0.212254	-0.632886	-0.318350
H	-0.535423	-1.432052	-0.340622
H	1.026410	-0.850258	0.382999

TS 8ttIN E = -311.981863 ν_i = -709

0 1

H	-2.133163	1.522896	-0.442363
C	-2.640174	0.587458	-0.175340
H	-4.443528	1.619086	0.375539
C	-3.925902	0.664364	0.287964
H	-4.482737	-0.231760	0.569319
C	-1.906311	-0.610356	-0.373447
H	-2.393681	-1.550642	-0.093360
C	-0.529096	-0.646940	-0.747466
H	-0.198354	-1.568534	-1.234091
H	-0.166329	0.242205	-1.272855
H	2.133143	1.522852	0.442473
C	2.640169	0.587441	0.175386
H	4.443520	1.619130	-0.375387
C	3.925902	0.664396	-0.287893
H	4.482753	-0.231701	-0.569306
C	1.906315	-0.610396	0.373391
H	2.393689	-1.550654	0.093223
C	0.529098	-0.647017	0.747404
H	0.198353	-1.568659	1.233936
H	0.166331	0.242076	1.272880

TS 8ttOUT E = -311.981904 ν_i = -708

0 1

H	-2.698281	-1.154402	0.892141
C	-2.889625	-0.261989	0.283411
H	-4.923256	-0.848037	-0.092209
C	-4.135550	-0.115231	-0.264316
H	-4.387152	0.751472	-0.878904
C	-1.820354	0.661433	0.157177
H	-1.990925	1.546112	-0.466005
C	-0.498847	0.422194	0.641349
H	0.107956	1.314677	0.814876
H	-0.430903	-0.282704	1.476602
H	2.698335	1.154415	-0.892066
C	2.889654	0.261953	-0.283402
H	4.923367	0.847838	0.092199
C	4.135584	0.115117	0.264306
H	4.387151	-0.751622	0.878880
C	1.820312	-0.661414	-0.157165
H	1.990891	-1.546216	0.465827
C	0.498817	-0.422063	-0.641330
H	0.430940	0.282937	-1.476513
H	-0.108068	-1.314469	-0.815003