

SUPPORTING INFORMATION

Isomerisation of *nido*-[C₂B₁₀H₁₂]²⁻ Dianions: Unprecedented Rearrangements and New Structural Motifs in Carborane Cluster Chemistry.

David McKay,* Stuart A. Macgregor and Alan J. Welch

Institute of Chemical Sciences, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, UK

Email: d.mckay@hw.ac.uk

Table of Contents

I. Additional isomerisation processes from 3,7.....	2
II. [B ₁₂ H ₁₂] ⁴⁺ <i>nido</i> , <i>inverted nido</i> and <i>basket</i> structures.	2
III. Computed geometries.	3

I. Additional isomerisation processes from 3,7.

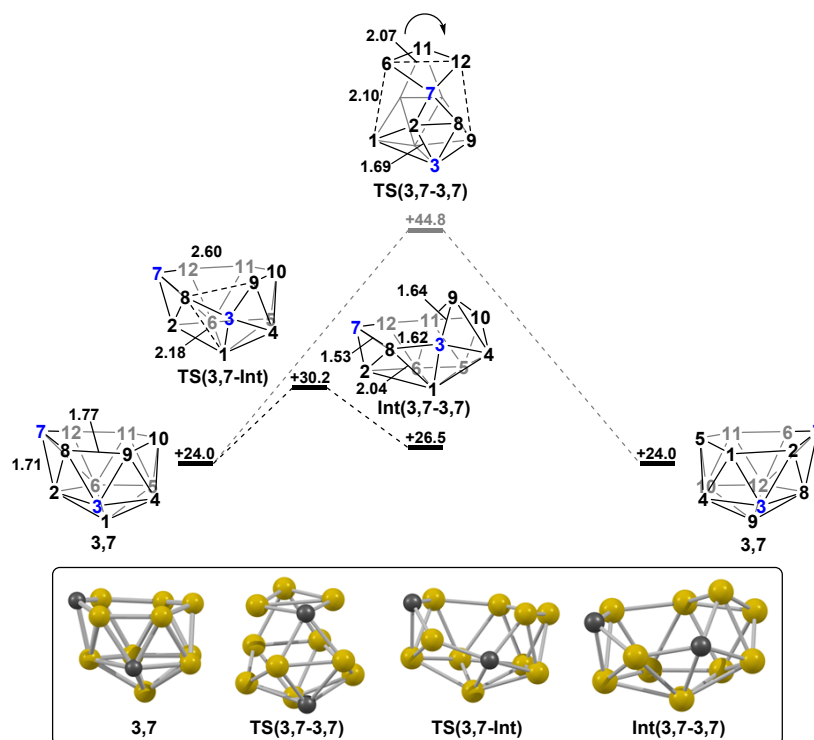


Figure S1. Degenerate pathways characterised from 3,7. Numbering of CH vertices (blue) and BH vertices (black) consistent with 3,7 (left). Inset shows computed structures. Selected distances in Å and energies relative to 7,9 in kcal/mol. H atoms omitted for clarity.

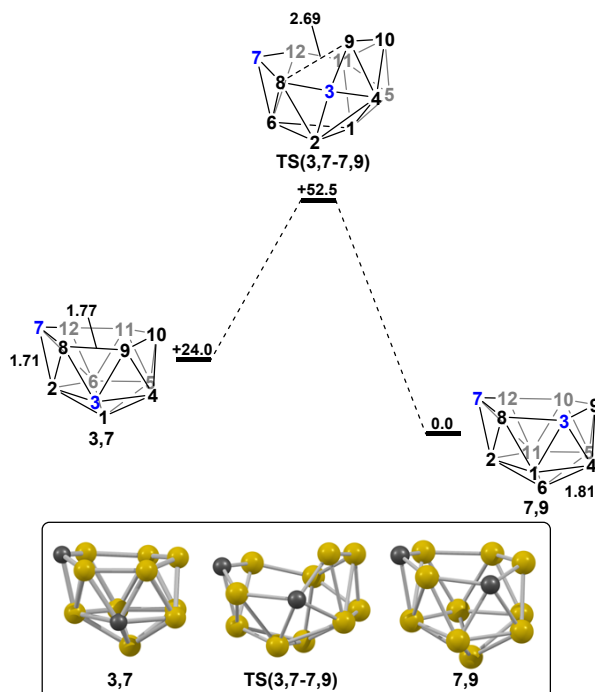
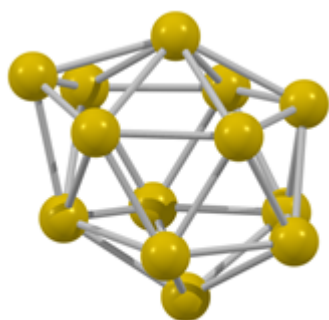
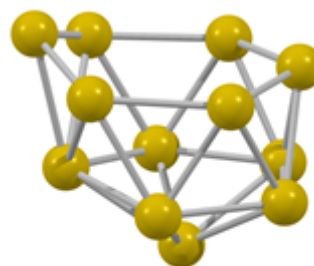


Figure S2. Formation of 7,9 from 3,7. Numbering of CH vertices (blue) and BH vertices (black) consistent with 3,7 (left). Inset shows computed structures. Selected distances in Å and energies relative to 7,9 in kcal/mol. H atoms omitted for clarity.

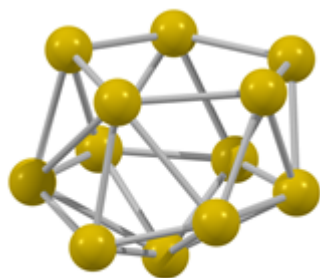
II. *closo*-[B₁₃H₁₃]²⁻, *nido*-[B₁₂H₁₂]⁴⁻ and *inverted nido* and *C*₂-*basket* tetraanion structures.



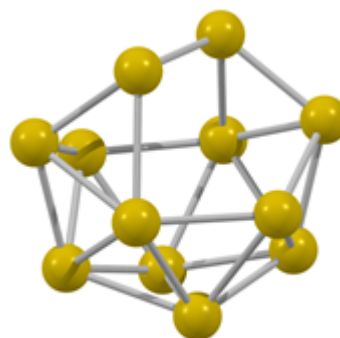
closo-[B₁₃H₁₃]²⁻



nido-[B₁₂H₁₂]⁴⁻



inverted nido



*C*₂-*basket*

III. Computed geometries.

ortho-carborane

SCF Energy = -332.070602164
Enthalpy 0K = -331.898039
Enthalpy 298K = -331.889084
Free Energy 298K = -331.928934
Lowest Frequencies = 451.5 453.7 cm⁻¹
C 0.00017 0.81523 -1.28330
B 1.46116 -0.00169 -0.85677
B 1.45643 0.00259 0.91635
B 0.89595 -1.44453 0.03092
C 0.00090 -0.82102 -1.28049
B -0.89511 -1.44526 0.03003
B -0.00053 -0.89120 1.47152
B -0.00091 0.89747 1.46660
B -0.89590 1.44518 0.02404
B 0.89516 1.44549 0.02475
B -1.46032 -0.00237 -0.85809
B -1.45727 0.00180 0.91497
H 2.34660 -0.00317 -1.65348
H 1.49053 -2.46555 -0.13529
H 0.00135 -1.30444 -2.25934
H 2.49300 0.00383 1.51100
H -1.48906 -2.46658 -0.13647
H 1.48969 2.46548 -0.14777
H -0.00062 -1.53968 2.47468
H 0.00066 1.29398 -2.26426
H -0.00140 1.55126 2.46743
H -1.49103 2.46473 -0.14892
H -2.34515 -0.00470 -1.65548
H -2.49421 0.00212 1.50900

meta-carborane

SCF Energy = -332.095017031
Enthalpy 0K = -331.921948
Enthalpy 298K = -331.913073
Free Energy 298K = -331.952799
Lowest Frequencies = 470.2 471.7 cm⁻¹
C 0.00005 -0.80480 1.30869
B -0.00003 0.90875 1.43683
B 0.89930 1.46605 0.00056
B -0.89943 1.46597 0.00058
B -1.45125 0.01761 0.88934
B -1.45126 0.01831 -0.88930
B -0.00006 0.90987 -1.43612
B 1.45124 0.01844 -0.88932
B 0.89731 -1.41530 -0.00056
B 1.45126 0.01774 0.88931
B -0.89718 -1.41538 -0.00054
C 0.00002 -0.80378 -1.30932
H -0.00004 1.40885 2.52012
H -1.54083 2.47405 0.00098
H -2.40967 -0.08389 1.59194
H 1.54061 2.47419 0.00095
H -2.40970 -0.08265 -1.59196
H 2.40971 -0.08367 1.59190
H -0.00009 1.41082 -2.51902
H 0.00009 -1.39549 2.22727
H 2.40968 -0.08243 -1.59201
H 1.43462 -2.47736 -0.00098

H -1.43440 -2.47749 -0.00096
H 0.00004 -1.39374 -2.22836

para-carborane

SCF Energy = -332.099505470
Enthalpy 0K = -331.926232
Enthalpy 298K = -331.917385
Free Energy 298K = -331.957068
Lowest Frequencies = 462.1 467.3 cm⁻¹
C -0.00910 -0.10732 -1.53184
B -1.30158 -0.85028 -0.68656
B -0.57464 -1.35360 0.85218
B -1.51523 0.16798 0.75118
B -1.16639 0.93187 -0.81222
B -0.35580 1.53007 0.64871
C 0.00910 0.10732 1.53184
B 1.16639 -0.93187 0.81222
B 1.51523 -0.16798 -0.75118
B 0.35580 -1.53007 -0.64871
B 0.57464 1.35360 -0.85218
B 1.30158 0.85028 0.68656
H -2.16494 -1.42323 -1.27628
H -2.51879 0.28863 1.38345
H -1.94017 1.54011 -1.48510
H -0.95473 -2.24137 1.55135
H -0.59085 2.55351 1.21330
H 0.59085 -2.55351 -1.21330
H 0.01556 0.18363 2.62153
H -0.01556 -0.18363 -2.62153
H 1.94017 -1.54011 1.48510
H 2.51879 -0.28863 -1.38345
H 0.95473 2.24137 -1.55135
H 2.16494 1.42323 1.27628

1,7

SCF Energy = -331.961143558
Enthalpy 0K = -331.798629
Enthalpy 298K = -331.788206
Free Energy 298K = -331.830772
Lowest Frequencies = 198.4 326.4 cm⁻¹
C -1.96764 0.00000 -0.53489
B -1.14854 -0.00000 0.98116
C 0.55417 -0.00000 1.29100
B 0.04887 1.51154 0.75082
B 1.58134 0.88958 0.17822
B 1.58134 -0.88958 0.17822
B 0.04887 -1.51154 0.75082
B -1.29481 -1.37724 -0.48308
B 0.42230 -1.54094 -0.95920
B 1.20712 0.00000 -1.36038
B 0.42230 1.54094 -0.95920
B -1.29481 1.37724 -0.48308
H 0.71796 2.63299 -1.43234
H -2.02909 2.36166 -0.40635
H -3.07205 0.00000 -0.43719
H -2.02909 -2.36166 -0.40636
H 0.71797 -2.63298 -1.43234
H 2.09719 -0.00000 -2.20689
H 0.80402 -0.00000 2.35719
H 0.00507 -2.38164 1.59845
H 2.58846 -1.41051 0.62235

H 2.58845 1.41051 0.62235
H -1.78302 -0.00000 2.01457
H 0.00507 2.38164 1.59845

3,7

SCF Energy = -331.970132834
Enthalpy 0K = -331.807336
Enthalpy 298K = -331.796952
Free Energy 298K = -331.839478
Lowest Frequencies = 206.0 278.4 cm⁻¹
C 1.96819 -0.07418 -0.50443
B 1.14383 -0.09274 0.98885
B -0.61378 0.00539 1.44352
C -0.14597 -1.39375 0.64320
B -1.62936 -0.78478 0.15643
B -1.53773 0.98524 0.23575
B 0.04615 1.49399 0.80575
B 1.36789 1.33127 -0.50079
B -0.34587 1.59884 -0.90307
B -1.19982 0.12468 -1.35608
B -0.49273 -1.45772 -1.01105
B 1.19588 -1.40947 -0.49202
H -0.85418 -2.56365 -1.39241
H 1.82311 -2.45594 -0.35302
H 3.06777 -0.17198 -0.42645
H 2.15119 2.28040 -0.45484
H -0.56558 2.71225 -1.36955
H -2.07143 0.17215 -2.22075
H -0.86337 -0.12811 2.62168
H 0.21456 2.40098 1.60113
H -2.54666 1.58616 0.56390
H -2.61400 -1.41224 0.49627
H 1.80076 -0.29578 1.98975
H -0.14781 -2.29015 1.27526

4,7

SCF Energy = -331.973596651
Enthalpy 0K = -331.810574
Enthalpy 298K = -331.800256
Free Energy 298K = -331.842647
Lowest Frequencies = 197.4 340.1 cm⁻¹
B -1.18074 0.04899 -1.36431
B -0.39347 1.56252 -0.93020
B 1.32439 1.36623 -0.47790
C 1.97190 -0.01678 -0.53006
B 1.26741 -1.38129 -0.48197
B -0.44303 -1.49168 -0.98684
C -1.44796 -0.78305 0.17498
B -1.54696 0.91827 0.21141
B -0.01362 1.51624 0.78685
B 1.15552 -0.06077 1.00760
B -0.05267 -1.50600 0.74258
B -0.58952 0.01356 1.45748
H -0.87868 -2.56108 -1.39434
H 1.97115 -2.38884 -0.42989
H 3.07742 -0.04633 -0.46531
H 2.07473 2.34057 -0.42008
H -0.68566 2.64648 -1.42220
H -2.16254 0.00942 -2.09964
H -0.96721 -0.07964 2.60350
H 0.08619 2.46219 1.54535

H -2.63118 1.37189 0.52380
H -2.38696 -1.29054 0.43416
H 1.87218 -0.10262 1.98921
H -0.14965 -2.49289 1.44233

7,8

SCF Energy = -331.989166729
Enthalpy 0K = -331.825521
Enthalpy 298K = -331.815400
Free Energy 298K = -331.857418
Lowest Frequencies = 217.7 340.6 cm⁻¹
C 1.68629 0.72651 -0.50543
C 1.68631 -0.72653 -0.50547
B 0.46808 -1.66731 -0.66887
B -1.08417 -0.85935 -1.21696
B -1.08411 0.85919 -1.21702
B 0.46813 1.66727 -0.66888
B -0.89976 1.46315 0.44734
B -1.85158 0.00003 0.16244
B -0.89980 -1.46316 0.44752
B 0.77557 -0.98263 1.02177
B -0.60771 -0.00002 1.46909
B 0.77544 0.98265 1.02165
H 0.77146 -2.84449 -0.83235
H 2.68876 -1.19484 -0.48975
H 2.68871 1.19487 -0.48939
H 0.77145 2.84452 -0.83190
H -1.75991 1.53403 -1.98721
H -1.76008 -1.53389 -1.98731
H -0.86418 0.00031 2.65693
H -1.41597 2.46903 0.90091
H -3.04058 0.00010 0.43288
H -1.41575 -2.46899 0.90148
H 1.39996 1.54371 1.90016
H 1.40002 -1.54337 1.90053

7,9

SCF Energy = -332.009355613
Enthalpy 0K = -331.845583
Enthalpy 298K = -331.835395
Free Energy 298K = -331.877620
Lowest Frequencies = 173.6 341.0 cm⁻¹
B 0.66249 0.09049 1.45877
B 0.22478 -1.46738 0.80603
B -1.09716 -0.13817 1.05423
B -0.08738 1.53010 0.77177
B 1.49234 1.06268 0.16542
B 1.66884 -0.69319 0.16920
B 0.22990 1.57871 -0.95146
B -1.45310 1.23671 -0.42875
B 1.08607 0.12349 -1.36458
C 0.50252 -1.35106 -0.85721
B -1.09547 -1.45465 -0.48257
C -1.96468 -0.19774 -0.47320
H 0.37676 2.66843 -1.49342
H -2.29129 2.13494 -0.35456
H -3.05285 -0.36411 -0.36117
H -1.61918 -2.56408 -0.50107
H 0.88692 -2.26898 -1.32979
H 1.88338 0.06459 -2.29427
H 0.96890 0.10291 2.63373

H	0.31822	-2.51135	1.41588
H	2.72769	-1.26705	0.33036
H	2.49242	1.71835	0.40261
H	-1.80391	-0.24855	2.03673
H	-0.27061	2.48378	1.50717

7,10

SCF Energy =	-332.007184866		
Enthalpy 0K =	-331.843384		
Enthalpy 298K =	-331.833260		
Free Energy 298K =	-331.875278		
Lowest Frequencies =	220.8 355.7 cm ⁻¹		
B	-0.65113	0.00000	1.47032
B	-0.05576	1.50967	0.77214
B	1.12790	-0.00000	1.03555
B	-0.05576	-1.50966	0.77214
B	-1.57943	-0.89035	0.20825
B	-1.57943	0.89035	0.20825
B	-0.38466	-1.45531	-0.96030
B	1.31430	-1.37222	-0.42448
C	-1.09806	-0.00000	-1.22591
B	-0.38466	1.45530	-0.96030
B	1.31430	1.37222	-0.42448
C	1.97872	0.00000	-0.50370
H	-0.73629	-2.43642	-1.60177
H	2.03622	-2.36398	-0.36958
H	3.08557	0.00000	-0.46067
H	2.03622	2.36398	-0.36958
H	-0.73630	2.43642	-1.60177
H	-1.87307	-0.00000	-2.01089
H	-0.95580	0.00000	2.64493
H	-0.00263	2.51011	1.46103
H	-2.65858	1.42591	0.36414
H	-2.65858	-1.42591	0.36414
H	1.85362	-0.00000	2.01126
H	-0.00262	-2.51011	1.46103

Int (A)

SCF Energy =	-331.951946177		
Enthalpy 0K =	-331.790122		
Enthalpy 298K =	-331.779568		
Free Energy 298K =	-331.822415		
Lowest Frequencies =	151.6 289.4 cm ⁻¹		
C	-0.58361	-1.15726	-0.80968
B	0.93576	-1.37564	-0.13848
B	2.02272	0.00444	-0.20030
B	0.90633	-0.21503	1.34514
B	-0.52662	-1.24538	0.92150
B	-1.01115	0.32833	1.51102
C	1.38874	1.16544	0.57991
B	0.31048	1.54325	-0.56076
B	-0.96154	0.50192	-1.25884
B	0.66658	-0.20910	-1.47939
B	-1.82750	-0.35932	0.06310
B	-1.40859	1.34068	0.20846
H	1.40519	-2.48168	-0.31201
H	1.49601	-0.60704	2.34302
H	-0.74103	-2.31481	1.45468
H	3.18761	-0.36608	-0.34640
H	-1.48011	0.30303	2.64070
H	0.95206	-0.49776	-2.62657

H	1.91814	1.92345	1.17768
H	-0.95562	-2.00706	-1.39275
H	0.57341	2.48013	-1.31809
H	-1.49924	0.67397	-2.33507
H	-2.91405	-0.89355	-0.07141
H	-2.30542	2.16754	0.10762

TS (A-1, 7)

SCF Energy =	-331.920420867		
Enthalpy 0K =	-331.759834		
Enthalpy 298K =	-331.749719		
Free Energy 298K =	-331.791697		
Lowest Frequencies =	-401.2 260.2 cm ⁻¹		
C	0.69363	-0.58847	1.22336
B	-0.67774	-1.38397	0.63427
B	-1.96247	-0.42502	-0.01594
B	-0.59844	-1.07819	-1.16601
B	0.87456	-1.51028	-0.21163
B	0.93596	-0.29568	-1.52068
C	-1.71104	0.89614	-0.64452
B	-0.45343	1.74695	-0.15388
B	0.81257	1.09637	0.94734
B	-0.77041	0.35414	1.28798
B	1.83296	-0.03660	0.01593
B	1.11168	1.34351	-0.79542
H	-1.04940	-2.34218	1.27992
H	-1.11626	-1.90432	-1.89942
H	1.38513	-2.60997	-0.09882
H	-3.03734	-1.00450	0.05623
H	1.59132	-0.65215	-2.49467
H	-1.25781	0.56026	2.37896
H	-2.53173	1.42626	-1.18943
H	1.10139	-1.00194	2.15092
H	-0.75751	2.90369	0.16402
H	1.27346	1.74095	1.86986
H	3.00755	-0.18712	0.29715
H	1.96949	2.16877	-1.09757

TS1 (A-4, 7)

SCF Energy =	-331.944172932		
Enthalpy 0K =	-331.783166		
Enthalpy 298K =	-331.772927		
Free Energy 298K =	-331.815450		
Lowest Frequencies =	-178.3 107.6 cm ⁻¹		
C	0.76484	1.56307	0.05015
B	-1.86838	0.80429	0.05910
B	-1.17527	-0.28519	-1.16251
B	-1.48903	-0.76738	0.58993
B	-0.60798	0.69280	1.32141
B	0.12022	-0.99698	1.29649
C	-0.22220	-1.48627	-0.32236
B	0.56891	-0.52195	-1.52396
B	1.75257	0.50170	-0.64641
B	-0.59827	1.48767	-0.80252
B	1.24841	0.34268	1.08504
B	1.38904	-1.06814	0.01699
H	-3.05763	1.07895	0.06401
H	-2.33170	-1.54125	1.00335
H	-0.77273	1.17920	2.42726
H	-1.91187	-0.73818	-2.02051
H	0.22118	-1.82679	2.17339

H -0.73268 2.31604 -1.70842
H -0.40182 -2.54916 -0.52029
H 1.10075 2.55003 0.41412
H 0.79334 -1.17250 -2.53376
H 2.93734 0.69132 -0.88240
H 2.02157 0.59470 1.98812
H 2.17731 -1.99075 0.06063

Int (A-4, 7)

SCF Energy = -331.944645640
Enthalpy 0K = -331.783515
Enthalpy 298K = -331.772460
Free Energy 298K = -331.816985
Lowest Frequencies = 47.6 214.4 cm⁻¹

C 0.51048 1.62500 -0.07073
B -2.00360 0.49310 0.02156
B -1.12191 -0.55604 -1.12602
B -1.32953 -0.88944 0.71376
B -0.63421 0.80821 1.16887
B 0.31037 -0.81893 1.37846
C -0.00743 -1.53700 -0.15560
B 0.62454 -0.65559 -1.49297
B 1.60313 0.64821 -0.78317
B -0.90714 1.38531 -0.80727
B 1.27451 0.59245 0.98677
B 1.54469 -0.88113 0.06556
H -3.21993 0.57704 0.03528
H -2.02972 -1.71521 1.26849
H -0.85574 1.41627 2.20092
H -1.82482 -1.21686 -1.87339
H 0.49685 -1.52041 2.34798
H -1.21074 2.22777 -1.65578
H -0.05697 -2.63062 -0.21572
H 0.75295 2.67607 0.16010
H 0.95445 -1.40664 -2.40014
H 2.69646 1.05479 -1.14630
H 2.01927 1.05506 1.82678
H 2.45545 -1.67606 0.18204

TS2 (A-4, 7)

SCF Energy = -331.944568273
Enthalpy 0K = -331.783591
Enthalpy 298K = -331.773342
Free Energy 298K = -331.815593
Lowest Frequencies = -85.6 221.3 cm⁻¹

C 0.47366 1.64340 -0.09570
B -2.01468 0.42516 0.00333
B -1.09135 -0.59417 -1.13946
B -1.30692 -0.92963 0.70714
B -0.66117 0.80290 1.15092
B 0.32481 -0.79434 1.38571
C 0.04022 -1.54579 -0.13595
B 0.65400 -0.67205 -1.48443
B 1.58230 0.67771 -0.79184
B -0.96049 1.39120 -0.78250
B 1.25047 0.63804 0.98283
B 1.56878 -0.84121 0.08150
H -3.23198 0.48786 0.00904
H -1.98643 -1.77041 1.26543
H -0.91158 1.41644 2.17258
H -1.78121 -1.28466 -1.87388

H 0.52115 -1.46991 2.37123
H -1.32279 2.25787 -1.58262
H 0.02233 -2.64148 -0.17643
H 0.70669 2.69950 0.12229
H 1.02315 -1.43119 -2.37012
H 2.66709 1.10861 -1.15417
H 1.97747 1.12761 1.82334
H 2.50407 -1.60399 0.21719

TS (1, 7-7, 9)

SCF Energy = -331.941151856
Enthalpy 0K = -331.779906
Enthalpy 298K = -331.769769
Free Energy 298K = -331.811843
Lowest Frequencies = -200.5 214.3 cm⁻¹

C -0.01576 1.72219 -0.17349
B 0.99695 0.97154 0.91621
C 0.47274 -0.56278 1.27661
B 1.76159 -0.39927 0.10780
B 0.54401 -1.66437 -0.05915
B -0.99103 -1.23143 0.69923
B -0.91997 0.65582 1.02754
B -1.40111 1.19488 -0.75536
B -2.02435 -0.15139 -0.11186
B -0.80095 -1.04967 -1.12405
B 0.90327 -0.60626 -1.44630
B 1.30196 1.01784 -0.85563
H 1.53037 -1.16299 -2.34065
H 2.21153 1.75318 -1.21978
H 0.01135 2.80808 0.01920
H -2.06766 2.02049 -1.38252
H -3.20885 -0.43604 -0.06918
H -1.34533 -1.87770 -1.84356
H 0.73272 -0.91027 2.28069
H -1.27069 1.14996 2.08223
H -1.47366 -2.07066 1.43582
H 0.89726 -2.80842 0.16465
H 1.50800 1.61754 1.80699
H 2.88119 -0.72803 0.45517

TS1 (4, 7-7, 10)

SCF Energy = -331.954896105
Enthalpy 0K = -331.792967
Enthalpy 298K = -331.782966
Free Energy 298K = -331.824900
Lowest Frequencies = -174.8 194.7 cm⁻¹

B 0.79136 1.20193 -1.09678
B 1.16130 -0.49407 -1.33272
B -0.13511 -1.60119 -0.88015
C -1.56280 -0.90392 -0.39657
B -1.90621 0.57873 -0.66975
B -0.78301 1.72028 -0.32744
C 0.57964 1.39001 0.57509
B 1.78304 0.32913 0.13127
B 1.18892 -1.32258 0.27876
B -0.47220 -1.33777 0.86771
B -1.12653 0.39632 0.95988
B 0.58389 -0.05841 1.44620
H -1.10302 2.89602 -0.21660
H -3.06944 0.90928 -0.88363
H -2.42209 -1.59501 -0.31544

H -0.26419 -2.75654 -1.27197
H 2.02693 -0.83357 -2.13461
H 1.34698 2.15366 -1.62912
H 0.88207 0.00003 2.61917
H 1.96365 -2.18949 0.64486
H 2.90860 0.65404 0.46230
H 0.89662 2.26525 1.15458
H -0.88074 -2.13858 1.68744
H -1.81369 0.65650 1.92700

Int1 (4,7-7,10)

SCF Energy = -331.961527507
Enthalpy 0K = -331.799425
Enthalpy 298K = -331.788855
Free Energy 298K = -331.831685
Lowest Frequencies = 202.6 226.3 cm⁻¹

B 1.17467 0.03992 -1.18002
B -0.03105 -1.31920 -1.25478
B -1.56757 -0.73145 -0.76496
C -1.51320 0.91029 -0.38405
B -0.16813 1.55028 -0.92394
B 1.23140 1.43858 -0.00693
C 1.72616 0.05038 0.50116
B 1.11546 -1.39407 0.08979
B -0.58157 -1.60633 0.44864
B -1.38029 -0.11649 0.94357
B -0.43702 1.38873 0.84759
B 0.34219 -0.34700 1.43996
H 2.02393 2.36480 -0.10106
H -0.22526 2.61367 -1.53010
H -2.44929 1.48298 -0.45316
H -2.67901 -1.16915 -1.04195
H 0.13230 -2.28830 -1.98927
H 2.10530 0.09775 -1.96951
H 0.55928 -0.51227 2.62335
H -0.92809 -2.67697 0.91406
H 1.90333 -2.30450 0.29464
H 2.74790 -0.03232 0.89336
H -2.24027 -0.10698 1.80435
H -0.71835 2.25249 1.65818

TS2 (4,7-7,10)

SCF Energy = -331.958281706
Enthalpy 0K = -331.797022
Enthalpy 298K = -331.786977
Free Energy 298K = -331.828823
Lowest Frequencies = -255.2 260.6 cm⁻¹

B -1.23992 -0.15683 -1.10551
B -0.07380 1.23146 -1.28143
B 1.51097 0.76724 -0.76619
C 1.60849 -0.81983 -0.27042
B 0.28475 -1.28669 -1.04877
B -1.07743 -1.55899 -0.00455
C -1.67853 -0.21639 0.59136
B -1.21471 1.28862 0.05517
B 0.45757 1.63532 0.40214
B 1.34867 0.19913 0.99079
B 0.50321 -1.39786 0.83830
B -0.38152 0.40998 1.46290
H -1.78442 -2.52773 -0.24627
H 0.44362 -2.11493 -1.93920

H 2.57591 -1.32421 -0.37791
H 2.57010 1.26013 -1.13058
H -0.27629 2.10344 -2.11431
H -2.15976 -0.28004 -1.89463
H -0.58002 0.67519 2.63304
H 0.75579 2.75840 0.76465
H -2.08101 2.13427 0.18986
H -2.70764 -0.18739 0.97326
H 2.20563 0.29542 1.84851
H 0.86939 -2.23210 1.65364

Int2 (4,7-7,10)

SCF Energy = -
331.981263472
Enthalpy 0K = -331.818656
Enthalpy 298K = -
331.808292
Free Energy 298K = -
331.850826
Lowest Frequencies = 168.5179 217.8323
cm⁻¹

B 1.24702 0.02387 -1.12448
B 0.21220 -1.43013 -0.88150
B -1.41100 -1.01082 -0.36730
C -1.66959 0.61629 -0.39871
B -0.50036 0.14895 -1.51379
B 0.73157 1.65124 -0.43571
C 1.66959 0.61629 0.39871
B 1.41100 -1.01082 0.36730
B -0.21220 -1.43013 0.88150
B -1.24702 0.02387 1.12448
B -0.73157 1.65124 0.43571
B 0.50036 0.14895 1.51379
H 1.26584 2.54169 -1.09966
H -0.78923 0.20441 -2.69739
H -2.72900 0.80887 -0.62243
H -2.36176 -1.72156 -0.63313
H 0.38517 -2.45394 -1.51496
H 2.10170 0.00726 -1.98865
H 0.78923 0.20440 2.69739
H -0.38517 -2.45394 1.51495
H 2.36176 -1.72157 0.63312
H 2.72900 0.80887 0.62243
H -2.10170 0.00725 1.98865
H -1.26584 2.54169 1.09967

TS3 (4,7-7,10)

SCF Energy = -331.975114257
Enthalpy 0K = -331.812969
Enthalpy 298K = -331.803058
Free Energy 298K = -331.844746
Lowest Frequencies = -236.2 227.4 cm⁻¹

B -1.13018 0.77221 0.98262
B -0.52419 -0.85549 1.33601
B 1.08485 -1.16972 0.66640
C 1.84804 0.10876 0.04099
B 0.64486 0.59810 1.25350
B -0.19584 1.84069 -0.10211
C -1.35830 0.86726 -0.70759
B -1.69502 -0.63541 0.00804
B -0.33855 -1.69681 -0.24304

B 0.98346 -0.79002 -1.15007
B 1.33643 1.37891 -0.64574
B -0.69733 -0.44099 -1.50345
H -0.47794 3.00461 0.18161
H 1.12684 1.02438 2.28427
H 2.93057 -0.05461 0.16067
H 1.82498 -1.96327 1.21590
H -0.82943 -1.42762 2.36272
H -1.88102 1.31922 1.76441
H -1.22306 -0.81813 -2.54243
H -0.50597 -2.89920 -0.34173
H -2.84804 -1.01704 0.06407
H -2.30597 1.31805 -1.04214
H 1.72289 -1.41545 -1.89241
H 2.18540 2.06551 -1.22612

TS1 (1,7-3,7)

SCF Energy = -331.933281850
Enthalpy 0K = -331.771307
Enthalpy 298K = -331.761550
Free Energy 298K = -331.802917
Lowest Frequencies = -154.0 287.0 cm⁻¹

C -0.64057 0.08731 1.28650
B 0.49239 -1.10694 0.99281
B -1.77087 0.37842 -0.00395
B -0.58150 1.60733 0.44472
B 0.87237 1.64624 -0.52025
B 0.93142 0.72932 1.01947
C 0.13413 -1.61421 -0.59437
B -1.20520 -1.23148 0.34692
B -1.01397 -0.60187 -1.31977
B -0.72081 1.11111 -1.25814
B 2.07106 0.44824 -0.52307
B 1.68074 -1.14231 -0.48394
H -0.99259 0.12154 2.32146
H 0.74319 -1.84345 1.91938
H -2.93195 0.57484 0.30383
H -1.01080 2.56438 1.06182
H 1.24992 2.81563 -0.54034
H 1.45627 1.04706 2.06943
H 0.04530 -2.70487 -0.73882
H -1.92380 -2.07692 0.83514
H -1.75505 -1.15509 -2.12282
H -1.29933 1.89181 -2.00662
H 3.23549 0.84287 -0.37911
H 2.44384 -2.10667 -0.35015

Int1 (1,7-3,7)

SCF Energy = -331.936090701
Enthalpy 0K = -331.773889
Enthalpy 298K = -331.763476
Free Energy 298K = -331.805996
Lowest Frequencies = 227.6 257.2 cm⁻¹

C 0.61897 -0.21229 1.28531
B 0.33237 1.36665 0.84449
B 1.33171 -1.21923 0.06610
B -0.28163 -1.53870 0.68177
B -1.65535 -1.07663 -0.30375
B -1.11060 0.18618 0.99226
C 0.64492 1.34246 -0.81556
B 1.72190 0.47949 0.15369

B 1.06710 -0.16348 -1.39662
B -0.02147 -1.48412 -1.06712
B -2.09912 0.47658 -0.60556
B -0.94043 1.64386 -0.38203
H 0.94694 -0.32393 2.32260
H 0.62527 2.23561 1.63500
H 2.23729 -1.96016 0.40197
H -0.39811 -2.45266 1.47628
H -2.49397 -1.95897 -0.12861
H -1.65509 0.32804 2.07248
H 1.17377 2.22866 -1.20280
H 2.81474 0.87340 0.49939
H 1.91365 -0.17817 -2.28218
H 0.02152 -2.55183 -1.66722
H -3.29473 0.78641 -0.62496
H -1.19698 2.83959 -0.23657

TS2 (1,7-3,7)

SCF Energy = -331.931795097
Enthalpy 0K = -331.770578
Enthalpy 298K = -331.760536
Free Energy 298K = -331.802439
Lowest Frequencies = -213.7 216.2 cm⁻¹

C 0.70733 -0.54694 1.23583
B 0.72562 1.08882 0.96270
B 0.88809 -1.51985 -0.13804
B -0.67386 -1.39281 0.68699
B -1.96259 -0.56197 -0.06465
B -1.04471 0.49249 1.04889
C 1.01650 1.19424 -0.72906
B 1.81448 -0.06596 0.05654
B 0.89849 -0.29761 -1.46862
B -0.60535 -1.14578 -1.14574
B -1.81285 0.95268 -0.65256
B -0.41212 1.79614 -0.20248
H 1.08662 -0.88568 2.20403
H 1.27235 1.79046 1.78725
H 1.47324 -2.57876 -0.01277
H -0.96503 -2.35262 1.37767
H -3.00496 -1.18117 0.09192
H -1.45729 0.75618 2.16875
H 1.77680 1.92228 -1.05468
H 3.00171 -0.05015 0.30183
H 1.61046 -0.51518 -2.43995
H -0.96201 -2.05979 -1.87907
H -2.81681 1.54263 -1.06476
H -0.43404 2.99721 0.06405

Int2 (1,7-3,7)

SCF Energy = -331.959765540
Enthalpy 0K = -331.798110
Enthalpy 298K = -331.787513
Free Energy 298K = -331.830327
Lowest Frequencies = 203.8 265.4 cm⁻¹

C -0.62493 -1.06499 -1.05996
B -0.71321 0.61546 -1.27330
B -0.37137 -1.58568 0.55678
B 0.91310 -1.48779 -0.66586
B 1.95020 -0.07658 -0.43856
B 1.02355 1.27194 -0.94717
C -1.57981 0.92050 0.25775

B	-1.74108	-0.61367	0.15630
B	-0.46906	0.11879	1.38142
B	1.14357	-0.78942	0.98304
B	1.20606	0.96075	0.81111
B	-0.24528	1.75850	0.13166
H	-1.15776	-1.74477	-1.74427
H	-1.37357	1.00110	-2.22688
H	-0.73818	-2.66948	0.96052
H	1.32296	-2.60149	-0.97489
H	3.17458	-0.14486	-0.47314
H	1.50758	2.29796	-1.41884
H	-2.45218	1.51549	0.55339
H	-2.83865	-1.12570	0.30376
H	-0.79938	0.21714	2.54349
H	1.72616	-1.30985	1.92141
H	1.83096	1.61254	1.63352
H	-0.45648	2.95744	0.25808

TS3 (1,7-3,7)

SCF Energy =	-331.949165653
Enthalpy 0K =	-331.788344
Enthalpy 298K =	-331.778116
Free Energy 298K =	-331.820308
Lowest Frequencies =	-296.9 254.8 cm ⁻¹

C	1.20247	-0.97194	-0.87853
B	-0.84235	-0.68588	-1.23923
B	1.42600	-0.67779	0.75837
B	1.75214	0.48473	-0.59235
B	0.52922	1.78678	-0.59563
B	-0.96590	1.09385	-1.12071
C	-1.29568	-1.24603	0.28330
B	0.16605	-1.76724	0.05335
B	-0.34659	-0.25707	1.37756
B	0.96496	1.00653	0.95578
B	-0.70591	1.48630	0.62450
B	-1.83891	0.22659	0.18621
H	1.86519	-1.72180	-1.34190
H	-1.25659	-1.36181	-2.16415
H	2.23905	-1.25596	1.45246
H	2.93999	0.69448	-0.81633
H	0.86292	2.95782	-0.74998
H	-1.78997	1.74156	-1.76495
H	-1.97715	-2.03465	0.61906
H	0.29204	-2.97893	0.14552
H	-0.58349	-0.49012	2.54367
H	1.52412	1.56071	1.89049
H	-1.21652	2.37719	1.28314
H	-3.03389	0.33539	0.43512

TS1 (7,10-7,9)

SCF Energy =	-331.963101809
Enthalpy 0K =	-331.801449
Enthalpy 298K =	-331.791543
Free Energy 298K =	-331.833164
Lowest Frequencies =	-377.3 273.7 cm ⁻¹

B	0.84573	-0.71384	1.31937
B	0.90362	-1.46998	-0.27796
B	-0.61696	-1.43469	0.61395
B	-0.70260	0.22815	1.40369
B	0.81011	1.06067	1.02758
B	1.83574	0.02121	0.02212

B	-0.52855	1.71906	-0.01113
B	-1.96424	-0.49870	0.03073
B	0.99030	1.37087	-0.74943
C	0.83544	-0.16117	-1.39015
B	-0.59330	-0.91449	-1.17875
C	-1.74605	0.83437	-0.56844
H	-0.87457	2.84786	0.34842
H	-3.01078	-1.13540	0.02589
H	-2.55193	1.34258	-1.15003
H	-1.00552	-1.65310	-2.05714
H	1.37831	-0.39000	-2.32038
H	1.81389	2.15584	-1.20307
H	1.35513	-1.24846	2.28386
H	1.45405	-2.52156	-0.53549
H	3.04657	-0.06945	-0.00843
H	1.27893	1.82109	1.85387
H	-1.01966	-2.48405	1.07690
H	-1.30007	0.45413	2.43634

Int (7,10-7,9)

SCF Energy =	-332.004225647
Enthalpy 0K =	-331.841043
Enthalpy 298K =	-331.830919
Free Energy 298K =	-331.872855
Lowest Frequencies =	268.8 294.3 cm ⁻¹

B	-0.71244	1.42209	-0.66861
B	-1.04503	-0.24022	-1.28095
B	0.56594	0.45602	-1.47615
B	0.92566	1.42616	-0.01444
B	-0.46557	1.14542	1.10857
B	-1.80563	0.35030	0.24341
B	0.99434	0.06272	1.29328
B	1.99758	0.06264	-0.29957
B	-0.78956	-0.54273	1.44411
C	-1.26023	-1.22519	0.06492
B	0.22531	-1.43710	-0.75136
C	1.40707	-1.22837	0.29623
H	1.64551	0.26217	2.30832
H	3.16992	0.40915	-0.41558
H	1.98266	-2.05358	0.74919
H	0.30306	-2.32614	-1.59818
H	-2.05624	-1.98013	-0.00089
H	-1.21213	-0.91994	2.52395
H	-1.18928	2.43982	-1.13323
H	-1.71451	-0.47961	-2.26614
H	-2.99080	0.59078	0.35614
H	-0.64308	2.01053	1.94512
H	0.87204	0.74176	-2.62089
H	1.49889	2.50007	-0.00611

TS2 (7,10-7,9)

SCF Energy =	-331.973457189
Enthalpy 0K =	-331.811445
Enthalpy 298K =	-331.801604
Free Energy 298K =	-331.843125
Lowest Frequencies =	-402.3 265.7 cm ⁻¹

B	-0.77175	-0.73002	1.33221
B	-0.86342	1.00748	1.01552
B	0.72886	0.30823	1.34708
B	0.72310	-1.40193	0.61342
B	-0.82342	-1.55113	-0.24936

B	-1.82823	-0.14224	0.01645
B	0.65994	-1.02537	-1.18093
B	1.98404	-0.38059	0.01269
B	-0.85633	-0.24898	-1.50922
C	-1.04749	1.18964	-0.68886
B	0.36502	1.71710	-0.11785
C	1.69193	0.96034	-0.55882
H	1.21579	-1.77698	-1.96614
H	3.10102	-0.87345	0.09533
H	2.52493	1.57394	-0.98684
H	0.48314	2.92334	0.10477
H	-1.80720	1.92565	-0.99668
H	-1.50492	-0.41737	-2.53368
H	-1.21272	-1.22338	2.34997
H	-1.40935	1.78329	1.77317
H	-3.04120	-0.14824	0.08412
H	-1.29709	-2.66744	-0.36318
H	1.28819	0.62249	2.37736
H	1.20374	-2.38445	1.14785

Int (B)

SCF Energy =	-331.979297522
Enthalpy 0K =	-331.816260
Enthalpy 298K =	-331.806040
Free Energy 298K =	-331.848261
Lowest Frequencies =	179.4 282.0 cm ⁻¹

C	0.61115	-1.52740	0.45416
B	-1.82739	-0.74682	0.11027
B	-1.47864	0.98717	0.02204
B	-0.85957	-0.09386	-1.34721
C	-0.61115	-1.52740	-0.45416
B	0.97240	0.11121	-1.48113
B	0.00312	1.43530	-0.90566
B	-0.00312	1.43530	0.90567
B	0.85957	-0.09386	1.34721
B	-0.97239	0.11121	1.48113
B	1.82738	-0.74682	-0.11027
B	1.47864	0.98717	-0.02204
H	-3.00389	-1.02955	-0.06541
H	-1.46967	-0.16904	-2.39926
H	-0.66529	-2.40765	-1.12590
H	-2.44441	1.72672	-0.02122
H	1.45861	0.13192	-2.59884
H	-1.45861	0.13192	2.59884
H	-0.12590	2.44705	-1.56929
H	0.66528	-2.40765	1.12590
H	0.12591	2.44705	1.56930
H	1.46967	-0.16904	2.39926
H	3.00389	-1.02956	0.06541
H	2.44441	1.72672	0.02123

TS (B-7, 9)

SCF Energy =	-331.921718590
Enthalpy 0K =	-331.761328
Enthalpy 298K =	-331.751185
Free Energy 298K =	-331.793222
Lowest Frequencies =	-484.5 224.5 cm ⁻¹

C	-1.53287	1.13986	-0.49554
B	0.70205	-0.10984	-1.56718
B	1.81087	-0.26421	-0.13233
B	0.63782	-1.54218	-0.47189

C	-0.77890	-0.72181	-1.07491
B	-0.78644	-1.34400	0.59748
B	0.79968	-0.95324	1.20406
B	1.03112	0.83668	1.05370
B	-0.23045	1.76571	0.13889
B	1.23782	1.30906	-0.67512
B	-1.96709	-0.14582	0.12330
B	-0.55403	0.17328	1.52334
H	1.01751	-0.41634	-2.71010
H	0.83191	-2.69225	-0.81446
H	-1.35487	-1.28426	-1.82222
H	2.99403	-0.55277	-0.16644
H	-1.38176	-2.35668	0.89784
H	2.14711	2.07853	-0.96288
H	1.28082	-1.66558	2.06302
H	-2.15122	1.70409	-1.23515
H	1.63997	1.42204	1.93323
H	-0.43919	2.90849	0.56340
H	-3.08940	-0.63727	0.07965
H	-1.03099	0.35650	2.62561

TS (B-7, 8)

SCF Energy =	-331.953085554
Enthalpy 0K =	-331.791556
Enthalpy 298K =	-331.781501
Free Energy 298K =	-331.823494
Lowest Frequencies =	-394.7 186.1 cm ⁻¹

C	-0.14266	1.75314	-0.09724
B	1.26507	1.27906	-0.59385
B	1.77445	-0.23223	0.22535
B	1.10268	-0.30792	-1.43100
C	-1.40770	1.12875	-0.60252
B	-0.53706	-0.88338	-1.32702
B	0.77020	-1.59753	-0.26247
B	0.51695	-0.85454	1.34471
B	-0.96379	0.05158	1.36581
B	0.66789	0.92053	1.14906
B	-1.92615	-0.21274	-0.22725
B	-0.88890	-1.45304	0.39954
H	2.17300	2.10065	-0.68072
H	1.83681	-0.58970	-2.37093
H	-2.06904	1.84213	-1.15536
H	2.94657	-0.38678	0.52053
H	-1.08105	-1.48924	-2.23678
H	1.07633	1.57386	2.09243
H	1.17169	-2.74478	-0.35936
H	-0.28555	2.82046	0.16096
H	0.85802	-1.35137	2.39961
H	-1.63941	0.36053	2.32346
H	-3.08975	-0.52000	-0.42231
H	-1.50209	-2.45601	0.71256

TS1 (7, 8-7, 9)

SCF Energy =	-331.963691133
Enthalpy 0K =	-331.801888
Enthalpy 298K =	-331.791809
Free Energy 298K =	-331.833908
Lowest Frequencies =	-74.9 166.8 cm ⁻¹

C	0.77972	1.58332	-0.00572
C	1.64620	0.48344	-0.53970
B	0.80054	-0.59520	-1.42823

B -0.98675 -0.35535 -1.30379
 B -1.93546 0.63250 -0.14349
 B -0.68224 1.56898 -0.67397
 B -0.92081 0.58412 1.26000
 B -1.53831 -0.92194 0.40533
 B -0.10555 -1.67776 -0.33835
 B 1.40934 -1.04315 0.22671
 B 0.01672 -0.95795 1.31792
 B 1.02946 0.49329 1.19080
 H 1.34379 -1.12389 -2.38790
 H 2.72936 0.67170 -0.63642
 H 1.27018 2.54911 0.20827
 H -1.00110 2.56700 -1.33533
 H -3.09423 0.96978 -0.30669
 H -1.63886 -0.72199 -2.27300
 H 0.10185 -1.58458 2.35596
 H -1.23450 1.13920 2.29830
 H -2.42884 -1.67522 0.75943
 H -0.20836 -2.87453 -0.54383
 H 1.78084 0.76771 2.10753
 H 2.38965 -1.72256 0.46150

Int1 (7,8-7,9)

SCF Energy = -331.963929768
 Enthalpy 0K = -331.801912
 Enthalpy 298K = -331.791148
 Free Energy 298K = -331.834865
 Lowest Frequencies = 92.1 145.7 cm⁻¹

C -0.51712 -1.58281 0.11174
 C -1.53311 -0.67690 -0.55862
 B -0.68795 0.35835 -1.51984
 B 1.09469 0.35947 -1.21835
 B 1.99726 -0.51148 0.08445
 B 0.89569 -1.47550 -0.67245
 B 0.72095 -0.48547 1.34006
 B 1.38258 1.02468 0.49824
 B 0.00277 1.63899 -0.46775
 B -1.51817 0.93641 0.00720
 B -0.25198 1.08666 1.23643
 B -1.13227 -0.42622 1.14404
 H -1.16550 0.69488 -2.59261
 H -2.55610 -1.04355 -0.73192
 H -0.86032 -2.56691 0.47693
 H 1.17121 -2.41680 -1.42561
 H 3.21160 -0.62562 0.11609
 H 1.78960 0.74319 -2.14840
 H -0.45888 1.81972 2.18309
 H 0.93822 -0.96242 2.44059
 H 2.17676 1.84457 0.92629
 H 0.04071 2.81768 -0.77209
 H -1.92106 -0.79562 1.98869
 H -2.58273 1.51974 0.06011

TS2 (7,8-7,9)

SCF Energy = -331.938593313
 Enthalpy 0K = -331.777905
 Enthalpy 298K = -331.767785
 Free Energy 298K = -331.809793
 Lowest Frequencies = -516.2 192.8 cm⁻¹
 C 1.49554 -0.94177 0.46009
 B -1.12255 -1.30850 0.68375

B -1.09155 0.39863 1.21507
 B -2.03414 -0.19549 -0.22277
 C -0.15904 -1.46420 -0.56848
 B -0.61791 -0.08376 -1.48760
 B -1.09844 1.27503 -0.38414
 B 0.28774 1.46559 0.76329
 B 1.76330 0.61103 0.19804
 B 0.55862 -0.21660 1.54498
 B 1.12911 -0.48589 -1.10157
 B 0.57907 1.22058 -0.98979
 H -1.42636 -2.25629 1.39674
 H -3.22108 -0.02359 -0.46565
 H -0.10780 -2.41738 -1.12941
 H -1.75225 0.76678 2.17183
 H -0.79217 -0.18738 -2.68913
 H 0.91340 -0.23763 2.71522
 H -1.72697 2.25806 -0.73050
 H 2.27463 -1.69847 0.60331
 H 0.41619 2.55342 1.29580
 H 2.88066 1.10410 0.15762
 H 1.80393 -0.91543 -2.01606
 H 0.95253 2.08646 -1.75573

Int2 (7,8-7,9)

See Int(7,10-7,9)

TS3 (7,8-7,9)

See TS2(7,10-7,9)

TS (3,7-3,7)

SCF Energy = -331.934314739
 Enthalpy 0K = -331.774163
 Enthalpy 298K = -331.763739
 Free Energy 298K = -331.806281
 Lowest Frequencies = -230.5 213.9 cm⁻¹
 C -0.78549 -1.50316 -0.00008
 B -1.51528 -0.36426 0.90431
 B -0.29219 0.74078 1.45378
 C -1.22407 1.03317 0.00025
 B 0.35322 1.64692 -0.00018
 B 1.41311 0.54327 0.90033
 B 0.52643 -1.14696 1.03725
 B 0.52619 -1.14722 -1.03708
 B 1.87990 -0.86794 -0.00005
 B 1.41243 0.54274 -0.90104
 B -0.29303 0.74076 -1.45382
 B -1.51607 -0.36409 -0.90378
 H -0.52048 1.45522 -2.41282
 H -2.60070 -0.52899 -1.42906
 H -1.17574 -2.52738 -0.00006
 H 0.53727 -1.82880 -2.05382
 H 3.04613 -1.22826 -0.00048
 H 2.22514 1.04587 -1.65797
 H -0.51948 1.45495 2.41302
 H 0.53756 -1.82845 2.05405
 H 2.22604 1.04697 1.65665
 H 0.42742 2.86000 -0.00025
 H -2.59937 -0.52936 1.43062
 H -1.99996 1.80821 0.00052

TS (3,7-Int)

SCF Energy = -331.959217340
 Enthalpy 0K = -331.797429
 Enthalpy 298K = -331.787258
 Free Energy 298K = -331.829513
 Lowest Frequencies = -103.8 236.0 cm⁻¹
 C 1.79925 -0.55661 -0.87596
 B 1.72743 -0.08437 0.71647
 B -0.09406 -0.35979 1.30971
 C -0.66664 -1.54460 0.16480
 B -1.79166 -0.37938 0.53903
 B -1.09535 1.20391 0.70027
 B 0.66702 1.27707 0.81579
 B 1.52304 0.99315 -0.74842
 B -0.16477 1.62845 -0.74633
 B -1.69390 0.68590 -0.89585
 B -1.38261 -0.93656 -1.11888
 B 0.94783 -1.58749 -0.15495
 H -1.82470 -1.70661 -1.95300
 H 1.39861 -2.70041 0.09161
 H 2.81056 -0.89122 -1.17113
 H 2.43579 1.76326 -1.03485
 H -0.26512 2.77876 -1.15756
 H -2.66939 1.25604 -1.36470
 H -0.14107 -0.71144 2.47070
 H 1.01557 2.11468 1.63687
 H -1.70904 1.98262 1.40882
 H -2.75319 -0.77848 1.16984
 H 2.63887 -0.17852 1.51826
 H -0.94740 -2.52590 0.56792

Int(3,7-3,7)

SCF Energy = -331.965582254
 Enthalpy 0K = -331.803330
 Enthalpy 298K = -331.792679
 Free Energy 298K = -331.835683
 Lowest Frequencies = 224.8 261.8 cm⁻¹
 C -2.03395 0.16919 -0.79382
 B -1.73882 -0.31946 0.75367
 B -0.06413 0.48298 1.25492
 C 0.22436 1.50340 -0.16067
 B 1.65128 0.91700 0.45281
 B 1.33891 -0.81692 0.91822
 B -0.33304 -1.30593 0.79207
 B -1.21704 -1.16727 -0.78742
 B 0.65586 -1.25495 -0.76712
 B 2.15723 -0.38729 -0.51726
 B 1.05772 0.62579 -1.26200
 B -1.38025 1.33870 -0.05301
 H 1.26493 1.13139 -2.35372
 H -1.99378 2.31812 0.35721
 H -3.10654 0.18208 -1.04707
 H -1.74748 -2.19997 -1.17800
 H 0.94606 -2.29563 -1.33709
 H 3.26862 -0.76429 -0.82543
 H -0.07345 0.96541 2.36907
 H -0.45773 -2.26977 1.53251
 H 1.93467 -1.41076 1.79708
 H 2.39091 1.71406 1.00345
 H -2.61210 -0.55802 1.56841
 H 0.40473 2.58862 -0.08385

TS(3,7-7,9)

SCF Energy = -331.922109206
 Enthalpy 0K = -331.761881
 Enthalpy 298K = -331.751035
 Free Energy 298K = -331.794717
 Lowest Frequencies = -163.1 169.0 cm⁻¹
 C 1.85607 0.38615 -0.86157
 B 1.50865 0.45797 0.77999
 B 0.51455 -0.90648 1.17447
 C -0.01205 -1.72086 -0.16027
 B -1.29522 -0.85857 0.62436
 B -1.80391 0.83808 0.54813
 B -0.28224 0.72892 1.31193
 B 0.97660 1.63153 -0.75410
 B -0.66209 1.71591 -0.29888
 B -1.71096 0.26106 -1.05533
 B -0.94441 -1.19669 -1.28766
 B 1.55293 -1.03530 -0.30160
 H -1.35275 -2.06582 -2.05735
 H 2.41608 -1.90024 -0.27416
 H 2.92688 0.55823 -1.07725
 H 1.57506 2.70631 -0.88533
 H -1.08718 2.86903 -0.24462
 H -2.74238 0.44839 -1.70582
 H 0.69464 -1.54460 2.19088
 H -0.29724 1.11747 2.46861
 H -2.79881 1.26317 1.10268
 H -2.00127 -1.61542 1.26983
 H 2.30820 0.79808 1.63106
 H 0.02505 -2.80847 0.00601

closo-[B₁₃H₁₃]²⁻

SCF Energy = -331.037636224
 Enthalpy 0K = -330.864230
 Enthalpy 298K = -330.853068
 Free Energy 298K = -330.897086
 Lowest Frequencies = 136.6 231.1 cm⁻¹
 B 2.11967 -0.00002 0.00000
 B 1.28200 -1.40077 0.00000
 B 1.28202 1.40076 0.00000
 B 0.84796 -0.00001 -1.35120
 B 0.84796 -0.00001 1.35120
 B -0.26945 -1.51102 -0.88396
 B -0.26943 1.51102 -0.88396
 B -0.26943 1.51102 0.88396
 B -0.26945 -1.51102 0.88396
 B -0.99001 0.00001 -1.43199
 B -0.99001 0.00001 1.43200
 B -1.65592 -0.89166 0.00000
 B -1.65590 0.89167 0.00000
 H 3.33424 -0.00003 0.00000
 H 1.92290 -2.43933 0.00000
 H 1.92293 2.43930 0.00000
 H 1.36105 -0.00001 -2.45318
 H 1.36105 -0.00001 2.45318
 H -0.35484 -2.51158 -1.56631
 H -0.35481 2.51158 -1.56631
 H -0.35481 2.51158 1.56631
 H -0.35484 -2.51158 1.56631
 H -1.54647 0.00001 -2.51095
 H -1.54647 0.00001 2.51095

H -2.71998 -1.47566 0.00000
H -2.71997 1.47569 0.00000

nido-[B₁₂H₁₂]⁴⁻

SCF Energy = -304.815809702
Enthalpy 0K = -304.669406
Enthalpy 298K = -304.658330
Free Energy 298K = -304.701938
Lowest Frequencies = 172.9 314.4 cm⁻¹
B 2.18089 0.00000 -0.61609
B 1.34769 -1.43233 -0.43239
B 1.34769 1.43233 -0.43239
B 1.16249 0.00000 0.97036
B -0.40119 -1.54151 -0.98738
B -0.40119 1.54151 -0.98738
B -0.03359 1.52126 0.75901
B -0.03359 -1.52127 0.75901
B -1.23583 0.00000 -1.37119
B -0.62590 0.00000 1.45566
B -1.58777 -0.89430 0.19349
B -1.58777 0.89431 0.19350
H 3.46308 -0.00000 -0.58539
H 2.00102 -2.51737 -0.27710
H 2.00102 2.51737 -0.27710
H 1.85422 -0.00000 2.00976
H -0.75918 -2.65157 -1.48054
H -0.75917 2.65157 -1.48054
H -0.01618 2.49818 1.53788
H -0.01619 -2.49818 1.53788
H -2.19035 0.00000 -2.20696
H -0.94354 0.00000 2.65814
H -2.64715 -1.47997 0.52143
H -2.64715 1.47997 0.52143

inverted nido-[B₁₂H₁₂]⁴⁻

SCF Energy = -304.771557386
Enthalpy 0K = -304.628354
Enthalpy 298K = -304.617051
Free Energy 298K = -304.661291
Lowest Frequencies = -220.0 116.8 cm⁻¹
B 2.03441 0.00000 0.32250
B 1.20053 -1.41115 0.12300
B 1.20053 1.41115 0.12300
B 1.03148 0.00000 -1.31222
B 0.46828 -0.00000 1.37388
B -0.13168 -1.49478 -1.10161
B -0.13168 1.49479 -1.10161
B -0.51276 1.51859 0.66256
B -0.51277 -1.51859 0.66256
B -1.36745 0.00000 0.99475
B -1.67976 -0.90423 -0.56220
B -1.67976 0.90423 -0.56220
H 3.23353 -0.00000 0.69641
H 1.87294 -2.47652 0.31401
H 1.87294 2.47652 0.31401
H 1.85782 0.00000 -2.26438
H 0.71088 -0.00000 2.59542
H -0.00617 -2.62242 -1.67395
H -0.00617 2.62242 -1.67395
H -0.73852 2.50640 1.39913
H -0.73852 -2.50640 1.39912

H -2.13679 -0.00000 1.98552
H -2.75944 -1.57459 -0.60167
H -2.75944 1.57459 -0.60166

basket-[B₁₂H₁₂]⁴⁻

SCF Energy = -304.784487828
Enthalpy 0K = -304.639785
Enthalpy 298K = -304.629056
Free Energy 298K = -304.672062
Lowest Frequencies = -97.3 172.1 cm⁻¹
B 1.12356 0.06021 -1.22782
B 0.13797 -1.44277 -0.89370
B -1.45868 -0.98163 -0.25296
B -1.85314 0.73627 -0.32689
B -0.67871 0.02735 -1.56595
B 0.75721 1.78467 -0.43718
B 1.85606 0.73015 0.32664
B 1.45392 -0.98638 0.25339
B -0.14414 -1.44187 0.89457
B -1.12379 0.06555 1.22744
B -0.74827 1.78646 0.43580
B 0.67845 0.02544 1.56599
H 1.10921 2.72020 -1.24840
H -1.00746 -0.09463 -2.77668
H -3.11914 0.81576 -0.39885
H -2.39731 -1.79623 -0.39569
H 0.28677 -2.51363 -1.52006
H 1.88791 -0.03560 -2.21758
H 1.00689 -0.09501 2.77673
H -0.29534 -2.51186 1.52180
H 2.38959 -1.80415 0.39700
H 3.12316 0.79989 0.39958
H -1.88851 -0.02512 2.21737
H -1.09799 2.72310 1.24807