Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1996, 35(21), 6170-6178, DOI:10.1021/ic960360g

Supporting Information to

The Existence of C,3-Me_2-*closo*-1,2-$C_2B_3H_3$ is Refuted by the *Ab Initio*/IGLO, GIAO-MP2/NMR Method. Attempted Repetition of the Synthesis

Matthias Hofmann, Mark A. Fox, Robert Greatrex, Paul von Ragué Schleyer, Joseph W. Bausch and Robert E. Williams

Cartesian coordinates of optimized geometries

1
1,2-*closo*-$C_2B_3H_5$ D_{3h} //RMP2(fc)/6-31G*

C	0.0000	0.0000	0.0000
C	1.5086	0.0000	0.0000
H	-0.5567	0.9339	0.0000
H	2.1841	0.8395	0.0000
B	-0.4056	-1.4586	-0.0000
B	0.9719	-1.0987	0.9140
B	0.9719	-1.0987	-0.9140
H	-1.4078	-2.0828	-0.0000
H	1.2394	-1.4582	2.0100
H	1.2394	-1.4582	-2.0100

1a
1,3-$(CH3)_2$-1,2-$C_2B_3H_3$ //RMP2(fc)/6-31G*

C	1.1334	0.0000	0.0000
C	0.0000	1.0003	0.0000
B	0.0000	-0.4869	-0.9047
B	0.0000	-0.4577	0.9286
B	-1.2682	0.1793	0.0239
C	2.6093	0.2170	-0.0010
C	-0.0204	-1.1072	-2.3525
H	0.2095	2.0688	-0.0013
H	-2.4339	0.3728	0.0108
H	-0.0073	-0.8875	2.0338
H	3.1224	-0.7479	0.0175
H	2.9342	0.7515	-0.8991
H	2.9344	0.7853	0.8755
H	0.5794	-2.0229	-2.3774
H	-1.0218	-1.3423	-2.7168
H	0.4425	-0.4046	-3.0547

1b
2,3-$(CH3)_2$-1,2-$C_2B_3H_3$ //RMP2(fc)/6-31G*

C	1.1210	0.0000	0.0000
C	0.0000	1.0074	0.0000
B	0.0000	-0.5024	-0.9053
B	0.0000	-0.4595	0.9436
B	-1.2603	0.1636	0.0319

C	0.2631	2.4868	-0.0086
C	-0.0397	-1.1489	-2.3409
H	2.1838	0.1863	0.0154
H	-2.4245	0.3728	0.0134
H	0.0039	-0.8929	2.0477
H	-0.6669	3.0574	-0.0097
H	0.8483	2.7620	0.8748
H	0.8481	2.7571	-0.8934
H	0.5607	-2.0643	-2.3554
H	-1.0465	-1.3915	-2.6847
H	0.4134	-0.4619	-3.0640

2

1,5-$C_2B_3H_5$ //RMP2(fc)/6-31G*

C	1.1313	0.0000	0.0000
B	0.0000	-0.5319	-0.9213
B	0.0000	-0.5319	0.9213
B	0.0000	1.0639	0.0000
C	-1.1313	0.0000	0.0000
H	0.0000	2.2497	-0.0000
H	0.0000	-1.1248	-1.9483
H	0.0000	-1.1248	1.9483
H	2.2097	0.0000	-0.0000
H	-2.2097	0.0000	0.0000

2a

1,2-Me_2-1,5-$C_2B_3H_3$ C_1 //RMP2(fc)/6-31G*

C	0.8194	-0.0347	-0.0000
B	-0.7228	0.2347	0.0000
B	0.1602	-1.1012	-0.9196
B	0.1603	-1.1012	0.9197
C	-1.0762	-1.2809	0.0001
C	2.0583	0.8051	-0.0001
C	-1.5848	1.5490	-0.0000
H	0.4940	-1.5964	-1.9463
H	0.4941	-1.5962	1.9464
H	-1.9722	-1.8817	0.0001
H	2.9570	0.1823	-0.0002
H	2.0970	1.4479	-0.8841
H	2.0972	1.4477	0.8840
H	-0.9790	2.4584	-0.0001
H	-2.2384	1.5726	-0.8780
H	-2.2383	1.5727	0.8781

2b

1,5-Me_2-1,5-$C_2B_3H_3$, D3H //RMP2(fc)/6-31G*

C	1.1423	0.0000	0.0000
B	0.0000	1.0557	0.0000
B	0.0000	-0.5278	-0.9142
B	0.0000	-0.5278	0.9142
C	-1.1423	0.0000	0.0000
C	2.6390	0.0000	-0.0000
C	-2.6390	0.0000	0.0000
H	0.0000	2.2433	-0.0000
H	0.0000	-1.1217	-1.9428
H	0.0000	-1.1217	1.9428
H	3.0308	-1.0206	-0.0000
H	3.0308	0.5103	-0.8839

H	3.0308	0.5103	0.8839
H	-3.0308	-1.0206	0.0000
H	-3.0308	0.5103	0.8839
H	-3.0308	0.5103	-0.8839

2c

2,3-Me_2-1,5-$C_2B_3H_3$, C2v //RMP2(fc)/6-31G*

C	0.0000	0.0000	-1.1264
B	1.0647	0.0000	0.0000
B	-0.5434	0.9319	0.0000
B	-0.5434	-0.9319	-0.0000
C	0.0000	0.0000	1.1264
C	-1.2922	2.3138	0.0000
C	-1.2922	-2.3138	-0.0000
H	2.2526	-0.0000	-0.0000
H	0.0017	0.0000	-2.2060
H	0.0017	0.0000	2.2060
H	-0.5455	3.1167	0.0000
H	-1.9135	2.4507	-0.8886
H	-1.9135	2.4507	0.8886
H	-0.5455	-3.1167	-0.0000
H	-1.9135	-2.4507	0.8886
H	-1.9135	-2.4507	-0.8886

3

1,2-$C_2B_4H_6$ //RMP2(fc)/6-31G*

C	0.0000	0.7677	0.0000
C	0.0000	-0.7677	-0.0000
B	0.7430	0.0000	-1.2160
B	1.6238	0.8555	0.0000
B	0.7430	0.0000	1.2160
B	1.6238	-0.8555	0.0000
H	-0.8587	1.4263	-0.0000
H	-0.8587	-1.4263	-0.0000
H	2.3451	1.7949	0.0000
H	2.3451	-1.7949	0.0000
H	0.5331	0.0000	-2.3799
H	0.5331	0.0000	2.3799

4

1,6-$C_2B_4H_6$ //RMP2(fc)/6-31G*

C	1.0821	0.0000	0.0000
B	0.0000	1.2086	0.0000
B	0.0000	0.0000	-1.2086
B	0.0000	-1.2086	-0.0000
B	0.0000	0.0000	1.2086
C	-1.0821	0.0000	0.0000
H	0.0000	2.3903	-0.0000
H	0.0000	0.0000	-2.3903
H	0.0000	-2.3903	-0.0000
H	0.0000	0.0000	2.3903
H	2.1654	0.0000	-0.0000
H	-2.1654	0.0000	0.0000

5

closo-2,3-$C_2B_5H_7$ //RMP2(fc)/6-31G*

B	1.3443	0.0000	1.1736
C	2.4072	0.7314	-0.0000
C	2.4072	-0.7314	-0.0000
B	0.9877	-1.3331	0.0000
B	0.0000	0.0000	0.0000
B	0.9877	1.3331	0.0000
B	1.3443	0.0000	-1.1736
H	-1.1862	0.0000	-0.0000
H	0.7872	2.5017	-0.0000
H	0.7872	-2.5017	0.0000
H	3.3487	1.2704	-0.0000
H	3.3487	-1.2704	-0.0000
H	1.5547	0.0000	-2.3405
H	1.5547	0.0000	2.3405

6

2,4-$C_2B_5H_7$ //RMP2(fc)/6-31G*

B	1.4152	0.0000	1.1593
C	0.9930	-1.1818	0.0000
B	0.0000	0.0000	0.0000
C	0.9930	1.1818	0.0000
B	2.5138	0.8244	-0.0000
B	2.5138	-0.8244	-0.0000
B	1.4152	0.0000	-1.1593
H	-1.1842	0.0000	-0.0000
H	0.6477	2.2093	-0.0000
H	0.6477	-2.2093	0.0000
H	3.3921	1.6203	-0.0000
H	3.3921	-1.6203	-0.0000
H	1.3117	0.0000	-2.3400
H	1.3117	0.0000	2.3400

7

closo-1,7-$C_2B_8H_8$ //RMP2(fc)/6-31G*

C	0.3858	0.0873	-1.2884
B	1.4596	-0.9685	-1.0629
B	1.7781	0.7720	-0.5865
B	0.0000	-0.9418	-0.0000
B	0.0000	0.9418	0.0000
B	1.7781	-0.7720	0.5865
C	0.3858	-0.0873	1.2884
B	1.4596	0.9685	1.0629
H	-0.8538	1.7661	0.0111
H	-0.8538	-1.7661	-0.0111
H	-0.1085	0.2998	-2.2298
H	-0.1085	-0.2998	2.2298
H	1.9269	-1.7042	-1.8661
H	1.9269	1.7042	1.8661
H	2.5339	-1.4260	1.2293
H	2.5339	1.4260	-1.2293

8

$C_2B_3H_5$ C1 //RMP2(fc)/6-31G*

B	-0.0473	-0.6635	-0.0914
C	-1.4617	-0.5928	-0.1066
B	-0.9720	0.7950	0.1855
B	0.7667	0.9168	-0.1168
C	1.4805	-0.4567	0.0998

H	1.7020	-0.7041	1.1416
H	2.2597	-0.7950	-0.5795
H	-2.4063	-1.1072	-0.1809
H	1.1631	1.8755	-0.7025
H	-1.5682	1.7858	0.4756

9

$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

B	0.9347	1.6079	0.0000
B	2.3209	1.2031	-0.5492
C	1.5557	0.0000	0.0000
B	0.0000	0.0000	0.0000
C	-0.5039	1.4344	0.4761
H	-0.6113	1.4161	1.5632
H	-1.3369	1.9372	-0.0102
H	3.4353	1.3343	-0.9213
H	-0.6375	-0.9295	-0.3912
H	2.0505	-0.9631	0.1405

10

$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

B	0.7440	1.4970	0.0000
B	2.2466	1.5938	-0.0835
B	1.5254	0.0000	0.0000
C	0.0000	0.0000	0.0000
C	-0.5685	1.0436	0.8467
H	-0.3495	1.0388	1.9086
H	-1.5427	1.4581	0.5929
H	3.3811	1.8867	-0.2198
H	-0.5899	-0.4266	-0.8130
H	2.2775	-0.8082	-0.4375

11

$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

B	1.3931	0.0000	0.0000
C	0.0000	0.0000	0.0000
B	0.1943	1.5401	0.0000
C	1.5107	2.2400	-0.6490
B	2.4809	1.2156	0.0297
H	3.4578	1.4439	0.6704
H	-0.9237	-0.5064	0.2239
H	-0.6531	2.1976	0.5312
H	1.4109	2.0618	-1.7239
H	1.6555	3.3035	-0.4495

12

$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

B	0.0000	0.0000	0.0000
B	1.5610	0.0000	0.0000
C	1.1022	1.4780	0.0000
C	0.0596	2.1668	0.8530
B	-0.8972	1.3057	-0.1005
H	-1.6445	1.7804	-0.8945
H	2.6055	-0.4211	-0.3629
H	1.6563	2.1051	-0.7027
H	0.1155	1.9044	1.9047
H	0.0078	3.2472	0.7125

13

$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

B	1.6516	1.7571	0.0000
B	2.8083	1.0600	0.7051
B	1.6326	0.0000	0.0000
C	0.0000	0.0000	0.0000
C	0.4847	1.1881	-0.7043
H	0.2397	1.3539	-1.7529
H	3.8654	0.7942	1.1565
H	-0.5335	-0.7542	-0.5762
H	2.2603	-0.8917	-0.4884
H	-0.3903	0.1420	1.0022

14

1,5-C2B3H5 C_{2v}, 2-B, mu(3,4)-H //RMP2(fc)/6-31G*

C	0.8194	1.1828	0.0000
B	0.0000	0.0000	0.0000
B	1.6308	0.0000	-0.8512
B	1.6308	0.0000	0.8512
C	0.8194	-1.1828	0.0000
H	2.0800	0.0000	-1.9473
H	0.9103	-2.2543	0.0000
H	0.9103	2.2543	0.0000
H	2.0800	0.0000	1.9473
H	2.6744	0.0000	-0.0000

15

$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

C	1.1250	1.0093	0.5750
B	1.8530	0.0000	0.0000
B	0.0000	0.0000	0.0000
C	-1.1746	1.0885	0.0000
B	-0.1811	1.5846	1.0899
H	-1.0574	1.6002	-0.9582
H	-2.2137	0.8408	0.2109
H	-0.0751	-1.1842	-0.1550
H	2.5615	-0.8234	-0.4473
H	-0.3821	1.9039	2.2223

16

$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

C	0.0000	0.0000	0.0000
B	-0.8465	0.9775	0.4826
B	0.8304	1.3500	0.0000
B	1.7835	0.0000	0.0000
C	0.8451	-1.0316	-0.7089
H	0.7740	-2.0615	-0.3584
H	0.6810	-0.9465	-1.7810
H	-1.7260	1.6539	0.8689
H	2.5564	-0.2560	0.8758
H	0.8543	2.5159	0.2058

17

$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

C	1.4366	0.0000	0.0000
B	2.4493	0.9569	0.0000
B	0.8151	1.4093	0.0000

C	0.0000	0.0000	0.0000
B	0.4618	3.0030	0.0002
H	-0.5288	-0.2698	0.9136
H	-0.5288	-0.2697	-0.9136
H	3.5353	1.4098	-0.0002
H	0.3292	3.6040	1.0245
H	0.3294	3.6044	-1.0239

18

$C_2B_3H_5$ C_s //RMP2(fc)/6-31G*

C	1.4405	0.0000	0.0000
B	2.4844	0.9191	-0.0000
B	0.8330	1.3977	0.0000
C	0.0000	0.0000	0.0000
B	3.9609	1.6727	-0.0000
H	-0.5227	-0.2846	0.9127
H	-0.5227	-0.2846	-0.9127
H	0.5246	2.5377	0.0000
H	4.5124	1.9639	1.0192
H	4.5124	1.9639	-1.0192

19

$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

C	1.4594	0.0000	0.0000
B	2.5239	0.8771	0.0157
B	0.8674	1.3974	0.0000
C	0.0000	0.0000	0.0000
B	-0.8272	-0.0060	-1.2899
H	-0.4762	-0.2349	0.9538
H	0.6350	2.5547	-0.0025
H	3.5853	1.3813	-0.0066
H	-2.0196	-0.0664	-1.2349
H	-0.2862	0.1329	-2.3473

20

nido-2,3,4-$C_3B_3H_7$ C_s //RMP2(fc)/6-31G*

B	1.0046	0.0000	1.1400
C	1.5036	1.1902	0.0000
C	2.2925	0.0000	-0.0193
C	1.5036	-1.1902	-0.0000
B	0.0000	-0.8828	-0.0000
B	0.0000	0.8828	0.0000
H	-0.9099	1.6213	0.1882
H	-0.9099	-1.6213	0.1882
H	1.9712	2.1317	0.2707
H	1.9712	-2.1317	0.2707
H	1.1333	0.0000	2.3149
H	3.3604	0.0000	0.1836
H	-0.2228	0.0000	-0.9555

21

2,5-(CH2)-*nido*-2,3-$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

B	0.0000	0.0000	0.0000
C	1.2288	-0.1325	1.1013
C	1.1392	-1.1816	0.0000
B	1.2032	-0.2950	-1.1929
B	1.1392	1.2265	0.0000
C	2.4450	0.7585	0.7587

H	3.2680	0.1841	0.3488
H	2.7708	1.4864	1.5063
H	1.3806	-0.3416	-2.3644
H	0.6904	2.3174	0.1597
H	0.9053	-0.2739	2.1319
H	1.0507	-2.2444	0.1933
H	-1.1781	0.0672	0.1224

21a

1-Me-2,5-(CH2)-*nido*-2,3-$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

B	0.0000	0.0000	0.0000
C	1.2293	-0.1203	1.1071
C	1.1549	-1.1723	0.0000
B	1.2291	-0.2792	-1.1859
B	1.1549	1.2252	0.0000
C	2.4489	0.7684	0.7892
C	-1.5650	0.0488	0.1367
H	3.2798	0.2011	0.3849
H	2.7587	1.4923	1.5477
H	1.3979	-0.3360	-2.3594
H	0.6897	2.3114	0.1544
H	0.8905	-0.2620	2.1334
H	1.0822	-2.2372	0.1929
H	-1.9100	-0.7408	0.8143
H	-1.9185	1.0071	0.5272
H	-2.0524	-0.1237	-0.8277

21b

4-Me-2,5-(CH2)-*nido*-2,3-$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

B	0.0000	0.0000	0.0000
C	1.2436	-0.1340	1.0942
C	1.1293	-1.1849	0.0000
B	1.1920	-0.3119	-1.2102
B	1.1293	1.2299	0.0000
C	2.4477	0.7590	0.7355
C	1.4587	-0.3540	-2.7485
H	3.2669	0.1878	0.3124
H	2.7841	1.4876	1.4777
H	0.6877	2.3242	0.1649
H	0.9260	-0.2762	2.1265
H	1.0215	-2.2448	0.2021
H	-1.1784	0.0670	0.1300
H	2.4724	0.0108	-2.9518
H	1.4041	-1.3773	-3.1330
H	0.7671	0.2734	-3.3163

21c

5-Me-2,5-(CH2)-*nido*-2,3-$C_2B_3H_5$ C_1 //MP2(fc)/6-31G*

B	0.0000	0.0000	0.0000
C	1.2288	-0.1499	1.0954
C	1.1338	-1.1954	0.0000
B	1.1638	-0.3267	-1.2052
B	1.1338	1.2422	0.0000
C	2.4394	0.7482	0.7393
C	0.5919	2.7199	0.1559
H	3.2605	0.1731	0.3253
H	2.7751	1.4681	1.4928
H	1.3316	-0.3766	-2.3781

H	0.9234	-0.3053	2.1301
H	1.0317	-2.2560	0.2003
H	-1.1778	0.0788	0.1285
H	1.1882	3.4012	-0.4619
H	-0.4574	2.8386	-0.1239
H	0.7070	3.0561	1.1932

22

nido-2,5-(CH2)-1,2-$C_2B_3H_5$ C_1 //RMP2(fc)/6-31G*

C	0.6379	0.5723	-0.6032
C	-0.3959	-0.6998	-0.5155
B	1.0250	-0.9879	0.0915
B	1.3647	0.4079	0.7926
B	-0.7815	0.9888	-0.0881
C	-1.4104	-0.2439	0.5941
H	-1.1630	-0.6740	1.5545
H	-2.4716	-0.3462	0.3591
H	0.9610	1.0032	-1.5492
H	-0.7607	-1.0952	-1.4616
H	-1.3820	1.8206	-0.6952
H	1.7923	-1.7376	-0.4312
H	1.9939	1.2137	1.3916

23

homo form of #8, 2,3-(CH2) bridged //RMP2(fc)/6-31G*

B	0.6295	1.3797	0.0000
C	1.1377	2.6714	-0.5025
C	2.4007	2.4996	-1.2340
B	2.3718	1.5584	0.1004
B	1.6194	0.0000	0.0000
C	0.0000	0.0000	0.0000
H	-0.3126	-0.5833	0.8658
H	-0.6457	-0.1770	-0.8602
H	3.1194	1.7419	1.0126
H	2.2615	-0.9221	0.3851
H	0.8649	3.6368	-0.0803
H	3.0857	3.3466	-1.2355
H	2.3697	1.9729	-2.1817

24

2,4,6-tribora-[3,1,0]-tricyclohexan //RMP2(fc)/6-31G*

C	2.1245	1.4263	-0.1599
B	1.5755	0.0000	0.0000
C	0.0000	0.0000	0.0000
B	-0.4022	1.5232	0.0000
C	0.8371	2.4177	-0.1600
B	1.7484	2.2698	1.0523
H	-0.5406	-0.7021	0.6423
H	-0.2456	-0.3189	-1.0336
H	0.8264	3.4114	-0.6093
H	2.2907	-0.9548	0.1102
H	-1.5078	1.9713	0.1099
H	3.0880	1.6694	-0.6091
H	2.1135	2.7440	2.0727

25
2,5,6-tribora-[2,1,1,0(5,6)]-tetracyclohexan //RMP2(fc)/6-31G*

C	-0.2112	1.5384	0.0000
C	0.0000	0.0000	0.0000
B	1.5998	0.0000	0.0000
C	2.1437	1.4439	-0.0002
B	0.9829	1.9575	0.9339
B	0.9828	1.9572	-0.9342
H	-0.4248	-0.4977	0.8815
H	-0.4248	-0.4977	-0.8815
H	1.0841	2.6506	-1.8989
H	2.3168	-0.9576	0.0001
H	-1.2138	1.9564	-0.0000
H	3.1999	1.6829	-0.0002
H	1.0844	2.6515	1.8982

A
1,2-C2B2H5 -> C1 TS //HF/6-31G*

C	0.0000	0.0000	0.0000
B	1.6374	0.0000	0.0000
C	1.0341	1.3192	0.0000
B	0.3324	1.2264	1.3802
B	-0.0277	-0.3813	1.4504
H	-0.5913	-0.2147	-0.8751
H	1.0083	2.1390	-0.6926
H	-0.4269	-1.3320	2.0248
H	-0.2473	2.1433	1.8694
H	2.5588	-0.7143	-0.1507

A
1,2-C2B2H5 -> Cs TS //Becke3LYP/6-311+G**

C	0.0000	0.0000	0.0000
B	0.9960	-0.3571	-1.1930
C	1.7605	0.0000	0.0000
B	1.2348	-0.9503	1.1024
B	-0.2405	-1.3858	0.5552
H	-0.5635	0.9300	0.0000
H	2.4246	0.8441	0.1638
H	-1.2185	-2.0447	0.6130
H	1.6047	-0.8623	2.2337
H	0.9611	-0.5456	-2.3546

B
C2B3H5, 1,3-ring C1 minimum //HF/6-31G*

C	0.0000	0.0000	0.0000
B	1.5317	0.0000	0.0000
C	1.1486	1.4386	0.0000
B	0.1601	1.8051	1.1196
B	-0.4748	0.2945	1.4332
H	-0.5526	-0.3691	-0.8499
H	1.4253	2.0999	-0.8100
H	-1.1587	-0.3760	2.1311
H	-0.2974	2.8983	1.2592
H	2.4177	-0.7400	-0.2405

B
TS from 1,2- to 1,5-C2B3H5 to 5-ring //RMP2(fc)/6-31G*

C	0.0000	0.0000	0.0000
B	1.5427	0.0000	0.0000
C	1.4776	1.5054	0.0000
B	0.1985	1.9414	0.7059
B	-0.4287	0.5439	1.3366
H	2.3410	-0.8575	-0.2017
H	-0.3715	2.9846	0.5619
H	-1.0469	0.0489	2.2199
H	2.0981	2.1409	-0.6419
H	-0.6011	-0.3831	-0.8244

B
C2B3H5, 1,3-ring C1 minimum //Becke3LYP/6-311+G**

C	0.0000	0.0000	0.0000
B	1.5500	0.0000	0.0000
C	1.1656	1.4290	0.0000
B	0.0763	1.7072	1.0495
B	-0.4352	0.2019	1.4483
H	-0.5553	-0.3442	-0.8698
H	1.4302	2.1196	-0.8022
H	-1.0436	-0.5242	2.1563
H	-0.5293	2.7355	1.0907
H	2.4214	-0.7699	-0.1945

C
C1 TS from 1,5-C2B3H5 to 5-ring //HF/6-31G*

C	0.0000	0.0000	0.0000
B	1.5326	0.0000	0.0000
C	1.5724	1.5049	0.0000
B	0.3215	2.0928	0.6479
B	-0.4689	0.7412	1.2451
H	2.3117	-0.8664	-0.2179
H	-0.0780	3.2079	0.5066
H	-1.1656	0.3444	2.1164
H	2.2959	2.0740	-0.5713
H	-0.6059	-0.4295	-0.7821

C
C1 TS from 1,5-C2B3H5 to 5-ring Becke3LYP/6-311+G**

C	0.0000	0.0000	0.0000
B	1.5396	0.0000	0.0000
C	1.3753	1.4845	0.0000
B	0.1935	1.8967	0.8790
B	-0.4665	0.4601	1.3620
H	2.3597	-0.8275	-0.2005
H	-0.3173	2.9759	0.8659
H	-1.1406	-0.1067	2.1527
H	1.8737	2.1356	-0.7230
H	-0.5739	-0.3521	-0.8546