

# Supporting Information

## Breaking the Plane: $B_5H_5$ is a Three-Dimensional Structure

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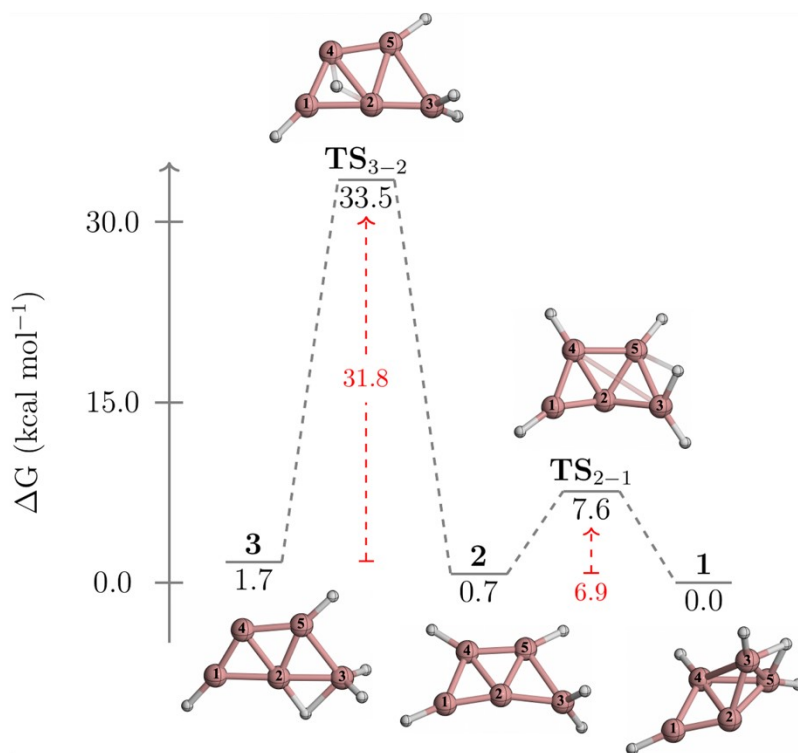
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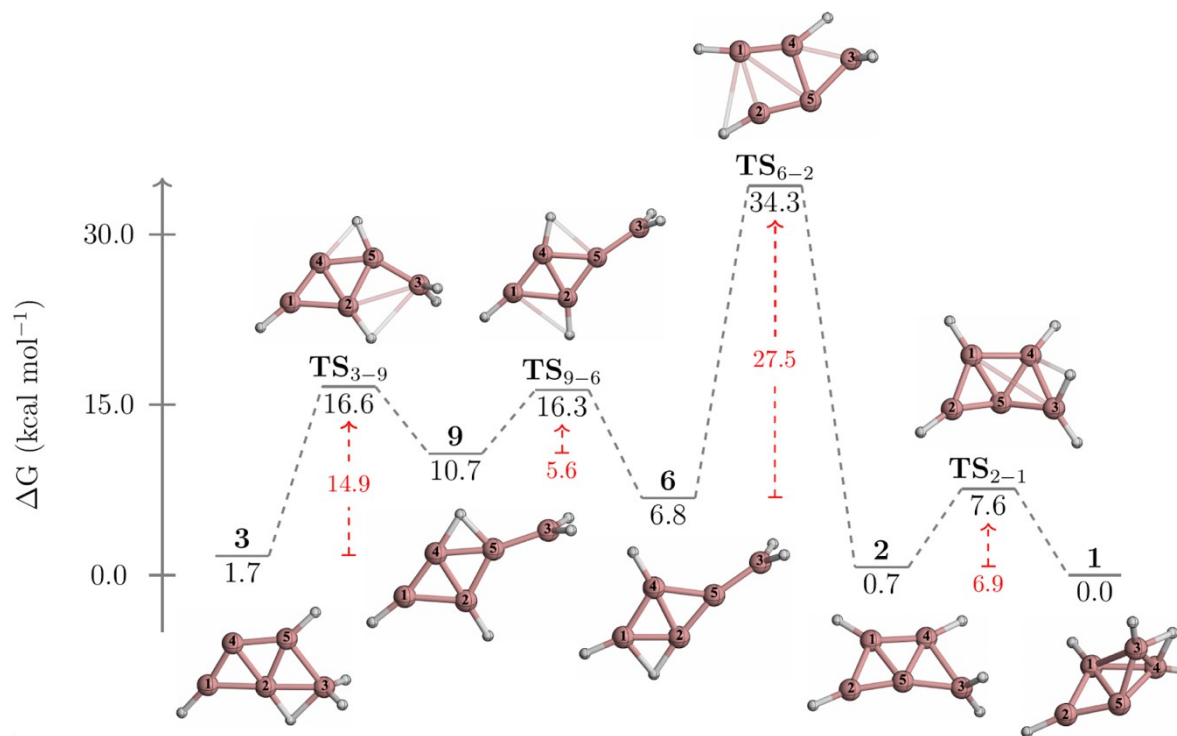
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**Figure S1.** Gibbs energy profile for converting **3** to **1**, with **2** acting as an intermediate, computed at the CCSD(T)/aug-cc-pVTZ//TPSS/def2-TZVP level of theory.



**Figure S2.** Gibbs energy profile for the transformation of **3** to **1** via a stepwise mechanism computed at the CCSD(T)/aug-cc-pVTZ//TPSS/def2-TZVP level of theory.

**Table S1.** T1 diagnostic values computed at the CCSD/aug-cc-pVTZ level of theory.

<b>Isomer</b>	<b>T1</b>
<b>1</b>	0.016
<b>2</b>	0.017
<b>3</b>	0.015
<b>4</b>	0.017
<b>5</b>	0.016
<b>6</b>	0.017
<b>7</b>	0.015
<b>8</b>	0.015
<b>9</b>	0.018
<b>10</b>	0.015
<b>11</b>	0.019
<b>12</b>	0.014
<b>13</b>	0.023
<b>14</b>	0.021

## Cartesian Coordinates

1

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.84440 a.u.

H	-2.272247000	0.637942000	1.033121000
B	0.000000000	0.467525000	0.000000000
B	1.046498000	-0.766147000	0.000000000
H	-2.272247000	0.637942000	-1.033121000
B	-0.526746000	-1.041237000	0.000000000
B	1.472562000	0.908938000	0.000000000
H	2.086120000	-1.335786000	0.000000000
B	-1.694141000	0.479891000	0.000000000
H	-1.496864000	-1.725293000	0.000000000
H	2.464375000	1.540350000	0.000000000

2

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.84034 a.u.

B	-0.278751000	0.388276000	-0.712519000
H	-2.847467000	0.224037000	0.004310000
B	-1.682486000	0.177770000	-0.167247000
B	-0.389074000	-0.648758000	0.590987000
H	-0.512873000	-1.453865000	1.453619000
B	1.087802000	-0.611565000	-0.373350000
B	0.939894000	0.848161000	0.321991000
H	1.252849000	1.792339000	0.959461000
H	2.007968000	0.144873000	0.170266000
H	1.712602000	-1.476802000	-0.886972000

3

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.84191 a.u.

B	-0.350160000	-1.099046000	0.000000000
B	1.181881000	-0.659470000	0.000000000
B	0.000000000	0.495686000	0.000000000
B	1.690572000	0.774680000	0.000000000
B	-1.683976000	0.177355000	0.000000000
H	-0.891687000	1.389385000	0.000000000
H	-1.033336000	-2.067457000	0.000000000
H	-2.285182000	0.225183000	1.031776000
H	-2.285182000	0.225183000	-1.031776000
H	2.303803000	1.781686000	0.000000000

4

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.83561 a.u.

H	0.842224000	1.828284000	-0.917665000
B	0.470971000	0.875286000	-0.323165000
H	2.790196000	-0.462773000	-0.168782000
B	0.131354000	-0.513267000	0.410540000
H	-1.739721000	-1.691000000	-0.943109000
B	-1.158643000	0.687529000	0.250832000
H	-1.640755000	1.499555000	0.975560000
B	-1.366492000	-0.766363000	-0.306554000
B	1.637677000	-0.287682000	0.001020000
H	1.173719000	-1.151579000	0.890631000

5

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.83112 a.u.

H	-0.675937000	-3.130616000	0.000000000
B	0.649921000	-0.782845000	0.000000000
B	0.568212000	2.323999000	0.000000000
H	0.800929000	2.911486000	1.020108000
B	-0.499565000	-1.966449000	0.000000000
B	-0.908697000	-0.433552000	0.000000000
H	0.800929000	2.911486000	-1.020108000
H	1.785102000	-1.117318000	0.000000000
B	0.000000000	0.818607000	0.000000000
H	-1.760381000	-1.373843000	0.000000000

6

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.83148 a.u.

H	0.517027000	-2.400809000	-0.000000000
B	-0.167441000	-1.418232000	-0.000000000
H	-1.355574000	-1.568718000	-0.000000000
B	0.789477000	-0.099190000	-0.000000000
H	0.107663000	2.550233000	0.000000000
B	-0.167441000	0.173272000	1.199363000
H	-0.810320000	0.203797000	2.184868000
B	0.183150000	1.373218000	0.000000000
B	-0.167441000	0.173272000	-1.199363000
H	-0.810320000	0.203797000	-2.184868000

7

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.83193 a.u.

H	0.000000000	0.000000000	2.205897000
B	0.000000000	1.196369000	-0.221088000
H	0.000000000	2.273076000	-0.712992000
B	0.000000000	0.000000000	1.013565000
H	-0.000000000	-2.273076000	-0.712992000
B	1.196369000	-0.000000000	-0.221088000
H	2.273076000	-0.000000000	-0.712992000
B	-0.000000000	-1.196369000	-0.221088000
B	-1.196369000	0.000000000	-0.221088000
H	-2.273076000	0.000000000	-0.712992000

8

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.82922 a.u.

H	1.007334000	1.635331000	-0.000000000
B	1.351045000	0.352223000	-0.000000000
H	2.505618000	0.137665000	-0.000000000
B	-0.094017000	0.854513000	0.000000000
H	-2.550461000	-0.339226000	0.000000000
B	-0.094017000	-0.394107000	1.049091000
H	0.268348000	-1.036934000	1.973140000
B	-1.368830000	-0.290502000	0.000000000
B	-0.094017000	-0.394107000	-1.049091000
H	0.268348000	-1.036934000	-1.973140000

9

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.82436 a.u.

H	1.353700000	0.680068000	0.000000000
B	0.954062000	-0.563212000	0.000000000
B	0.585220000	-2.036200000	0.000000000
H	0.616574000	-3.213211000	0.000000000
B	-0.626919000	-0.808930000	0.000000000
H	-1.796011000	-0.994195000	0.000000000
H	-0.857991000	2.821106000	1.022847000
H	-0.857991000	2.821106000	-1.022847000
B	-0.604019000	2.253489000	0.000000000
B	0.000000000	0.731877000	0.000000000

10

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.81449 a.u.

B	-1.063832000	-0.220834000	0.000000000
H	1.385519000	2.648226000	1.020881000
B	0.000000000	0.863136000	0.000000000
B	1.004198000	2.150538000	0.000000000
H	1.385519000	2.648226000	-1.020881000
B	0.459265000	-0.875206000	0.000000000
B	-1.007618000	-1.777722000	0.000000000
H	-1.602608000	-2.800670000	0.000000000
H	0.227143000	-2.193614000	0.000000000
H	1.644360000	-1.001729000	0.000000000

**11**

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.81492 a.u.

B	-1.812988000	-0.348014000	-0.054888000
H	-2.658809000	-1.166543000	-0.060218000
H	-1.681295000	0.443845000	0.981391000
B	1.648325000	-0.525201000	0.020755000
H	2.755950000	-0.919480000	-0.001950000
H	0.759059000	-1.601769000	-0.011585000
H	1.601182000	1.761556000	0.013691000
B	-0.876361000	0.817513000	-0.167737000
B	0.800614000	0.888950000	0.019860000
B	0.085192000	-0.536770000	-0.002256000

**12**

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.81265 a.u.

B	-0.401311000	-0.943809000	-0.356389000
B	1.132888000	0.637016000	-0.438505000
H	2.032620000	1.011317000	-1.110304000
H	0.316254000	1.584973000	-0.341411000
B	0.983203000	-0.823347000	0.331461000
H	1.901095000	-1.370469000	0.841204000
H	-0.504231000	1.382114000	1.457095000
H	-2.786456000	0.263218000	-0.120344000
B	-1.669224000	-0.095572000	-0.234944000
B	-0.237412000	0.651482000	0.553129000

**13**

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP



G = -126.80911 a.u.

H	0.00000000	2.23465300	0.00300000
B	0.00000000	0.00000000	1.35093200
H	0.00000000	0.00000000	2.52926800
B	0.00000000	1.04626800	-0.00064100
H	0.00000000	0.00000000	-2.52919500
B	-0.90609500	-0.52313400	-0.00064100
H	-1.93526600	-1.11732600	0.00300000
B	0.00000000	0.00000000	-1.35082400
B	0.90609500	-0.52313400	-0.00064100
H	1.93526600	-1.11732600	0.00300000

**14**

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.78052 a.u.

H	-2.47562200	-0.38242600	-0.14163300
B	-1.33054400	-0.09300700	-0.18165000
H	-1.34549700	1.18268800	0.19524500
B	0.05832700	-0.40638100	-1.00627700
H	2.53232800	0.23151300	-0.10037400
B	0.11809500	-0.77383200	0.68425800
H	0.16808400	-1.56227100	1.56774400
B	1.38258400	-0.00039600	-0.21753400
B	-0.05961000	0.96815400	0.29096500
H	0.27644700	2.05780700	0.63020700

**a) Ts<sub>3-1</sub>**

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = - 126.80018 a.u.

H	-2.6450750	-0.2072860	0.0132090
B	0.0936100	-0.5122340	-0.3379490
B	0.8407370	0.8882780	0.3666440
H	-1.4088140	-1.5555870	0.9224650
B	-0.6210230	1.0388190	-0.1660660
B	1.7866580	-0.2809250	0.0751800
H	2.7045060	-0.9699100	-0.1915140
B	-1.5467970	-0.6166190	0.1972980
H	-1.4649610	1.7522000	-0.5793500
H	0.0484180	-1.6060120	-0.8403430

**b) Ts<sub>2-1</sub>**

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.83002 a.u.

B	0.0735070	-0.4070000	-0.4918120
B	-1.4218800	-0.7229160	0.1419950
H	-2.0807220	-1.6900510	-0.0436000
B	1.4985210	-0.7250630	0.0747470
H	2.4003200	-1.4553550	0.2830010
H	1.5474060	1.8523520	0.1906120
B	-0.7798730	0.8969710	-0.1038700
H	-1.8442580	0.0563940	0.9913080
B	0.9274780	0.8416770	0.1397270
H	-1.5115110	1.8183130	-0.2252570

**b) Ts<sub>4-2</sub>**

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = -126.82625 a.u.

H	1.1530480	1.9107430	-0.5327250
B	0.5713200	0.9528730	-0.1602750
H	2.6451220	-0.5018380	-0.5955920
B	0.0488020	-0.4544490	0.3356810
H	-2.0818050	-1.6911350	-0.6445360
B	-1.1009780	0.7595750	0.1122680
H	-1.7541470	1.6346070	0.5871250
B	-1.4260550	-0.8037900	-0.2240670
B	1.6188290	-0.4748000	-0.0121680
H	1.4781960	-1.2494180	0.9285370

**b) Ts<sub>7-4</sub>**

CCSD(T)/aug-cc-pvtz//TPSS/def2-TZVP

G = - 126.82903 a.u.

H	-1.4137250	0.2188720	1.2774880
B	0.0260150	-1.0347030	-0.3291380
H	-0.1224030	-1.9441010	-1.0704050
B	-0.1524130	0.0974760	0.8194690
H	0.2515460	2.0153060	-1.0569750
B	-1.4287930	0.0118220	-0.0317460
H	-2.4791920	0.1473490	-0.5405080
B	0.4192720	1.0631260	-0.3766710

B	1.3882370	-0.1457900	0.1118920
H	2.5021890	-0.3970870	0.4213660