Supporting information

Electronic excitations of 1,4-disilyl substituted 1,4-disilabicycloalkanes: A MS-CASPT2 study of the influence of cage size

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Figure I: Homodesmotic reaction scheme for calculating ring strain in 1a, 1b, 2a and 2b.

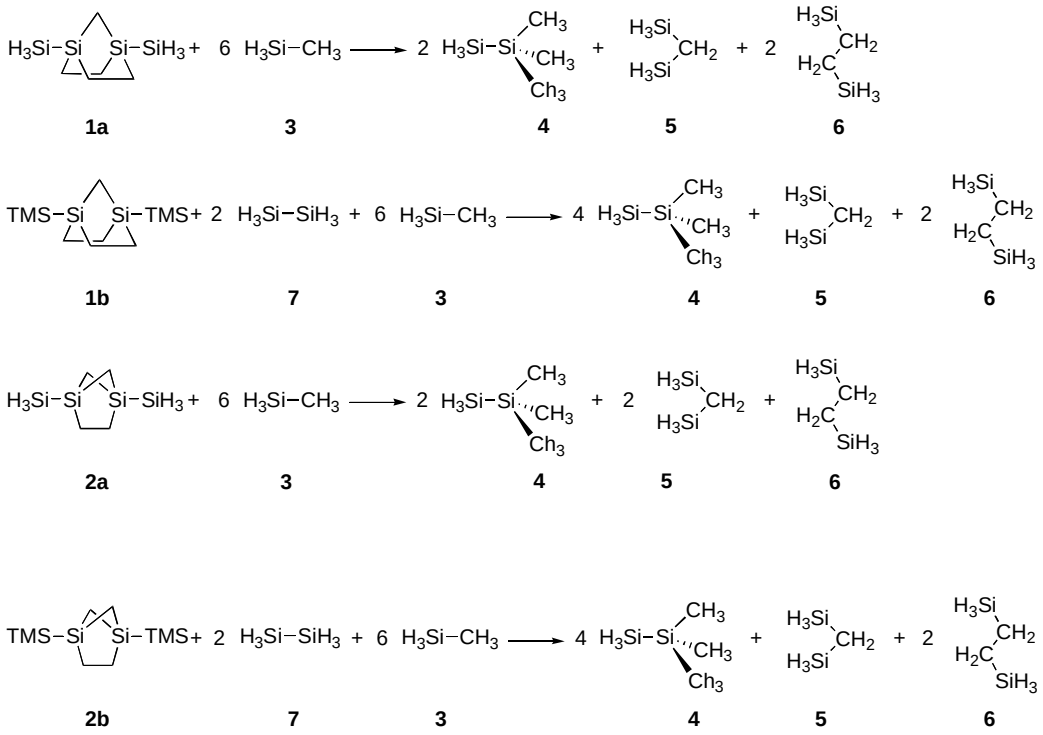

Table I: Absolute energies (in a.u.) for compounds 1 to 7 at MP2/cc-pVTZ level.

compound	Abs. E
1a	-1355.875647
1b	-1591.301992
2a	-1316.640528
2b	-1552.068007
3	-330.6407532
4	-699.3482482
5	-620.8740885
6	-660.0874958
7	-581.6352940

All geometries obtained at MP2/cc-pVTZ level of theory.
All molecules belong to the C_{2V} symmetry point group.

1a

C	-1.510674	0.784027	-1.023495
Si	0.000000	1.355334	-0.011489
H	1.465429	1.175636	-2.040366
H	-0.892336	0.000000	1.940797
Si	0.000000	3.603001	0.667708
H	-2.434613	1.163206	-0.585016
C	-1.510674	-0.784027	-1.023495
H	-1.465429	1.175636	-2.040366
Si	0.000000	-1.355334	-0.011489
H	-1.465429	-1.175636	-2.040366
H	-2.434613	-1.163206	-0.585016
Si	0.000000	-3.603001	0.667708
C	0.000000	0.000000	1.314439
C	1.510674	-0.784027	-1.023495
H	2.434613	-1.163206	-0.585016
C	1.510674	0.784027	-1.023495
H	1.465429	-1.175636	-2.040366
H	2.434613	1.163206	-0.585016
H	0.892336	0.000000	1.940797
H	-1.202911	3.897661	1.483043
H	0.000000	4.511943	-0.504566
H	1.202911	3.897661	1.483043
H	-1.202911	-3.897661	1.483043
H	1.202911	-3.897661	1.483043
H	0.000000	-4.511943	-0.504566

1b

C	0.000000	0.000000	1.030568
Si	0.000000	1.366125	-0.289916
C	-1.507215	0.783676	-1.308541
C	-1.507215	-0.783676	-1.308541
Si	0.000000	-1.366125	-0.289916
Si	0.000000	-3.615972	0.390365
C	1.507215	-0.783676	-1.308541
C	1.507215	0.783676	-1.308541
Si	0.000000	3.615972	0.390365
H	-1.457715	-1.175135	-2.326022
H	0.892266	0.000000	1.658363
H	2.4347	-1.163373	-0.876268
H	1.457715	-1.175135	-2.326022
H	1.457715	1.175135	-2.326022
H	2.4347	1.163373	-0.876268
H	-2.4347	1.163373	-0.876268
H	-1.457715	1.175135	-2.326022
H	-2.4347	-1.163373	-0.876268
H	-0.892266	0.000000	1.658363
C	1.540463	-3.959225	1.42671
C	0.000000	-4.749539	-1.12051
C	-1.540463	-3.959225	1.42671
C	1.540463	3.959225	1.42671
C	-1.540463	3.959225	1.42671
C	0.000000	4.749539	-1.12051

H	-1.557769	-4.998422	1.759099
H	-1.567299	-3.322619	2.311125
H	-2.449376	-3.775474	0.853569
H	1.557769	-4.998422	1.759099
H	2.449376	-3.775474	0.853569
H	1.567299	-3.322619	2.311125
H	0.000000	-5.797357	-0.815709
H	-0.881291	-4.580053	-1.739306
H	0.881291	-4.580053	-1.739306
H	0.000000	5.797357	-0.815709
H	0.881291	4.580053	-1.739306
H	-0.881291	4.580053	-1.739306
H	1.557769	4.998422	1.759099
H	1.567299	3.322619	2.311125
H	2.449376	3.775474	0.853569
H	-1.557769	4.998422	1.759099
H	-2.449376	3.775474	0.853569
H	-1.567299	3.322619	2.311125

2a

C	-1.313979	0.000000	-0.605492
Si	0.000000	1.241392	0.011762
Si	0.000000	3.508201	-0.5995
C	0.000000	0.783275	1.862223
C	0.000000	-0.783275	1.862223
Si	0.000000	-1.241392	0.011762
C	1.313979	0.000000	-0.605492
Si	0.000000	-3.508201	-0.5995
H	-0.877481	-1.17662	2.374932
H	0.877481	-1.17662	2.374932
H	0.877481	1.17662	2.374932
H	-0.877481	1.17662	2.374932
H	1.203604	-4.187365	-0.063075
H	0.000000	-3.638913	-2.075364
H	-1.203604	-4.187365	-0.063075
H	-1.379514	0.000000	-1.694904
H	-2.308585	0.000000	-0.165507
H	2.308585	0.000000	-0.165507
H	1.379514	0.000000	-1.694904
H	0.000000	3.638913	-2.075364
H	1.203604	4.187365	-0.063075
H	-1.203604	4.187365	-0.063075

2b

C	1.314349	0.000000	0.327965
Si	0.000000	1.24964	-0.284348
C	-1.314349	0.000000	0.327965
Si	0.000000	-1.24964	-0.284348
C	0.000000	-0.782774	-2.13703
C	0.000000	0.782774	-2.13703
Si	0.000000	-3.516651	0.339118
Si	0.000000	3.516651	0.339118
H	0.877428	-1.176697	-2.650782
H	-0.877428	1.176697	-2.650782
H	-0.877428	-1.176697	-2.650782
H	0.877428	1.176697	-2.650782
H	2.308892	0.000000	-0.113883
H	-2.308892	0.000000	-0.113883

H	1.382713	0.000000	1.417901
H	-1.382713	0.000000	1.417901
C	0.000000	-3.633195	2.222597
C	0.000000	3.633195	2.222597
C	1.542413	-4.362062	-0.346742
C	-1.542413	4.362062	-0.346742
C	-1.542413	-4.362062	-0.346742
C	1.542413	4.362062	-0.346742
H	0.000000	4.675809	2.544268
H	-0.881541	3.15032	2.644231
H	0.881541	3.15032	2.644231
H	-1.568627	5.411925	-0.050531
H	-1.562811	4.31941	-1.435689
H	-2.448803	3.884452	0.025087
H	1.568627	5.411925	-0.050531
H	2.448803	3.884452	0.025087
H	1.562811	4.31941	-1.435689
H	-1.568627	-5.411925	-0.050531
H	-2.448803	-3.884452	0.025087
H	-1.562811	-4.31941	-1.435689
H	0.000000	-4.675809	2.544268
H	0.881541	-3.15032	2.644231
H	-0.881541	-3.15032	2.644231
H	1.568627	-5.411925	-0.050531
H	1.562811	-4.31941	-1.435689
H	2.448803	-3.884452	0.025087