Supplementary Information

Can an eight π-electron bare ring be planar?

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1. Structures and Energies

All structures have been optimized at the B3LYP/def2-TZVPP level. All the energy values include the ZPE correction.

C4Si4H8
E = -1315.194055

Si	1.625294	1.625294	0.000000
C	0.000000	2.274484	0.000000
Si	-1.625294	1.625294	0.000000
C	-2.274484	0.000000	0.000000
Si	-1.625294	-1.625294	0.000000
C	0.000000	-2.274484	0.000000
Si	1.625294	-1.625294	0.000000
C	2.274484	0.000000	0.000000
H	-2.670821	2.670821	0.000000
H	-3.362538	0.000000	0.000000
H	-2.670821	-2.670821	0.000000
H	0.000000	-3.362538	0.000000
H	2.670821	-2.670821	0.000000
H	3.362538	0.000000	0.000000
H	2.670821	2.670821	0.000000
H	0.000000	3.362538	0.000000

C4Ge5H8
E = -8465.251794

Ge	1.694935	1.694935	0.000000
C	0.000000	2.395711	0.000000
Ge	-1.694935	1.694935	0.000000
C	-2.395711	0.000000	0.000000
Ge	-1.694935	-1.694935	0.000000
C	0.000000	-2.395711	0.000000

Ge	1.694935	-1.694935	0.000000
C	2.395711	0.000000	0.000000
H	-2.783201	2.783201	0.000000
H	-3.479764	0.000000	0.000000
H	-2.783201	-2.783201	0.000000
H	0.000000	-3.479764	0.000000
H	2.783201	-2.783201	0.000000
H	3.479764	0.000000	0.000000
H	2.783201	2.783201	0.000000
H	0.000000	3.479764	0.000000

C4SnH8
E = -1014.462543

Sn	1.867878	1.867878	0.000000
C	0.000000	2.640056	0.000000
Sn	-1.867878	1.867878	0.000000
C	-2.640056	0.000000	0.000000
Sn	-1.867878	-1.867878	0.000000
C	0.000000	-2.640056	0.000000
Sn	1.867878	-1.867878	0.000000
C	2.640056	0.000000	0.000000
H	0.000000	3.724359	0.000000
H	-3.083821	3.083821	0.000000
H	0.000000	-3.724359	0.000000
H	3.083821	-3.083821	0.000000
H	-3.724359	0.000000	0.000000
H	-3.083821	-3.083821	0.000000
H	3.083821	3.083821	0.000000
H	3.724359	0.000000	0.000000

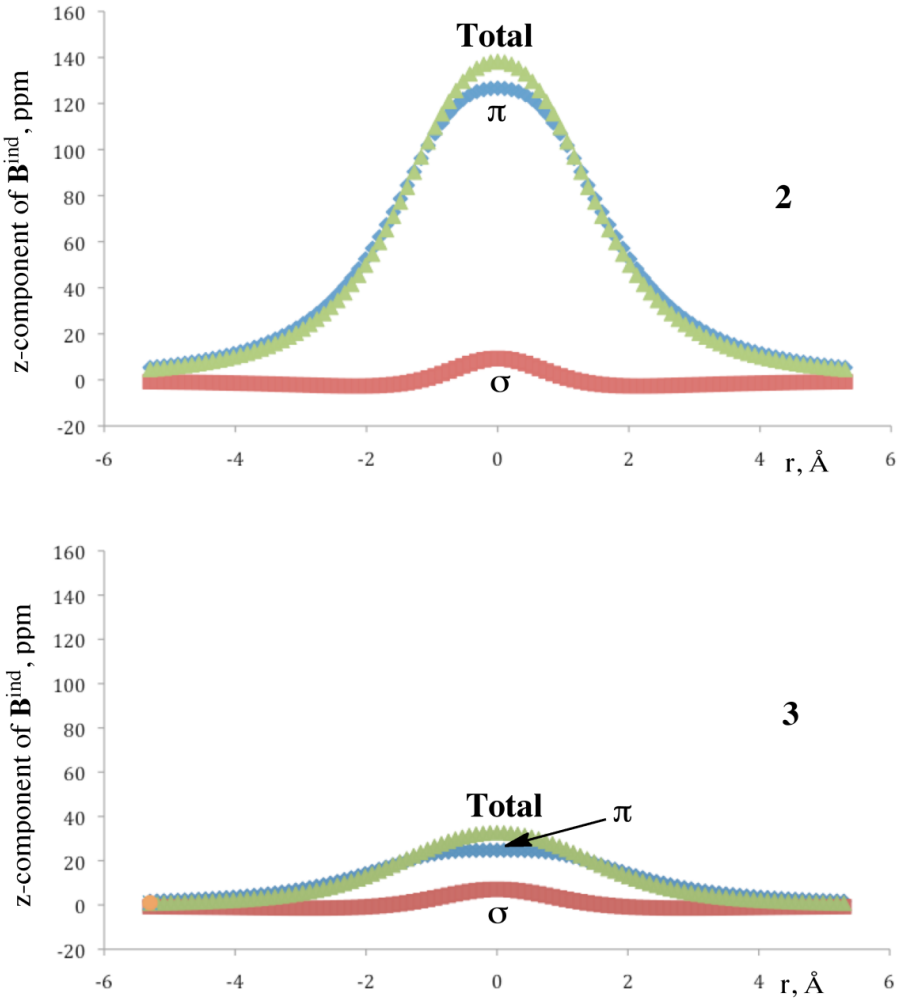

Figure 1-SI. B^{ind}_z profiles, including the orbital contributions, of **2**, **3**, and **4**

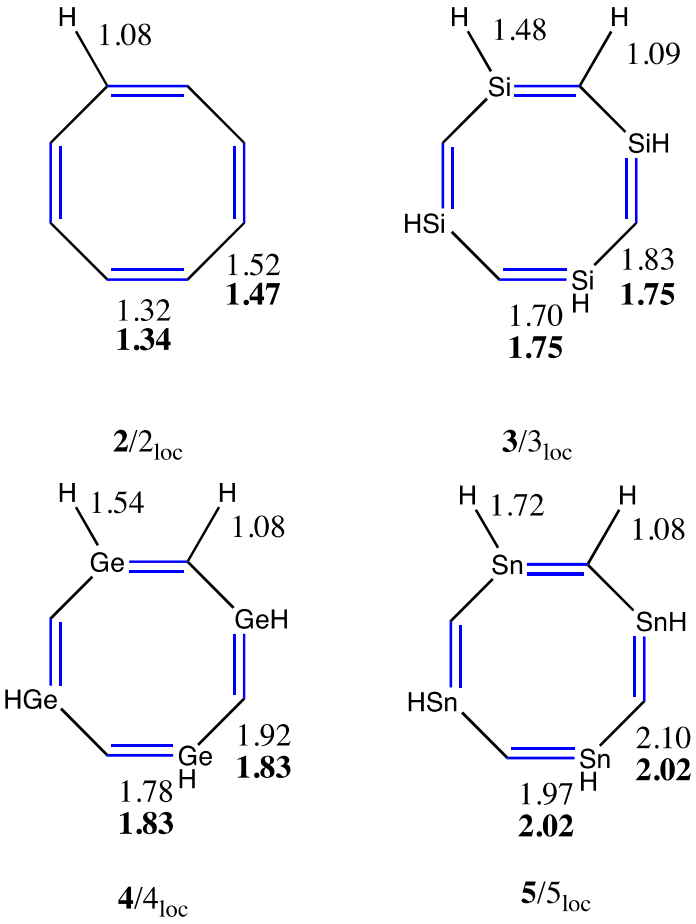

Figure 2-SI. (BLW)-B3LYP/def2-TZVPP bond lengths are given in Angstrom for **2**, **3** **4** and the optimized localized Lewis structures 2_{loc}, 3_{loc} and 4_{loc}. The block-double bonds are indicated in blue.