

Supporting Information

Borataalkene or Boratabenzene? Understanding the Aromaticity of 9-borataphenanthrene Anion and its Central Ring

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Figure S1. Reactions used for the calculation of isomerization stabilization energies.

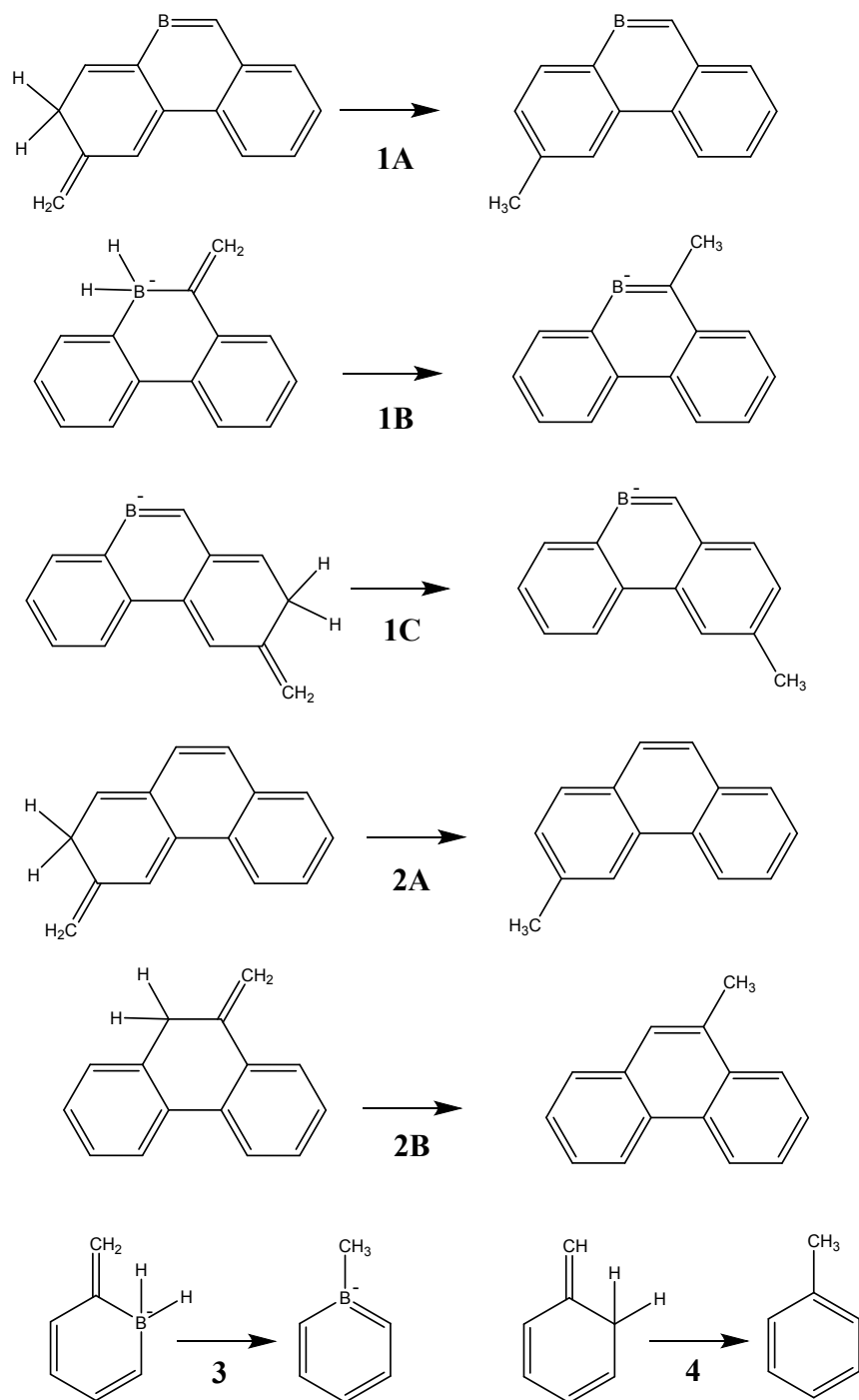


Figure S2. NICS_{zz} isolines for **4** at the B3LYP/6-311G**.

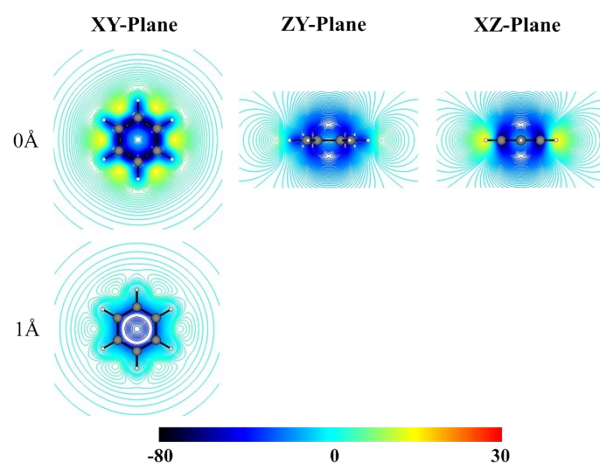


Figure S3. NICS_{zz} isolines for **3** at the B3LYP/6-311G**.

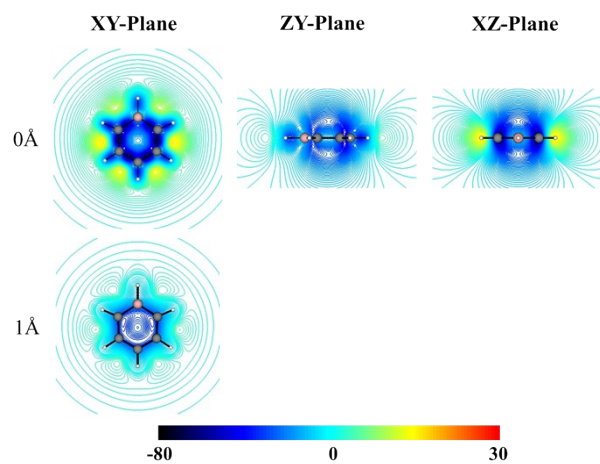


Figure S4. Canonical π -orbitals and their respective energies for **1** and **2** at the B3LYP/6-311G** level.

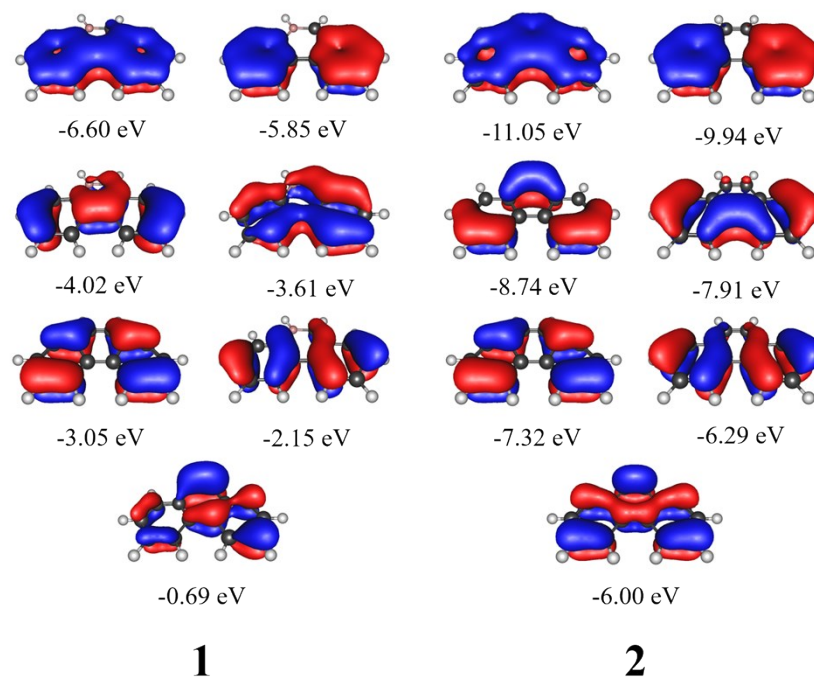


Figure S5. NICS_{zz} isosurfaces at most aromatic ring bifurcation value for **1** (-46 ppm) and **2** (-48 ppm), obtained at the B3LYP/6-311G** level.

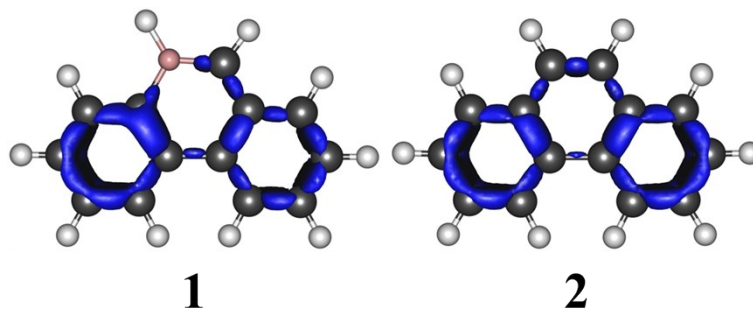


Figure S6. Orbital-Weighted Dual Descriptor ($f_w^{(2)}$) isosurfaces at 0.004 isovalue, obtained at the B3LYP/6-311G** level.

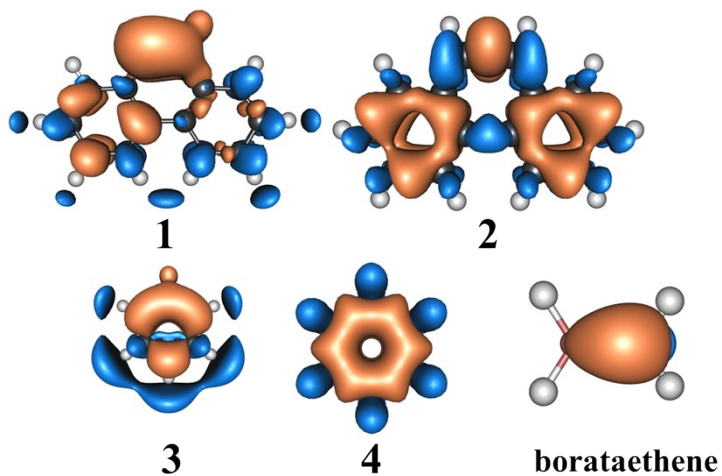


Figure S7. Localized σ -orbitals recovered from the AdNDP analysis of **1** at the B3LYP/6-311G** level.

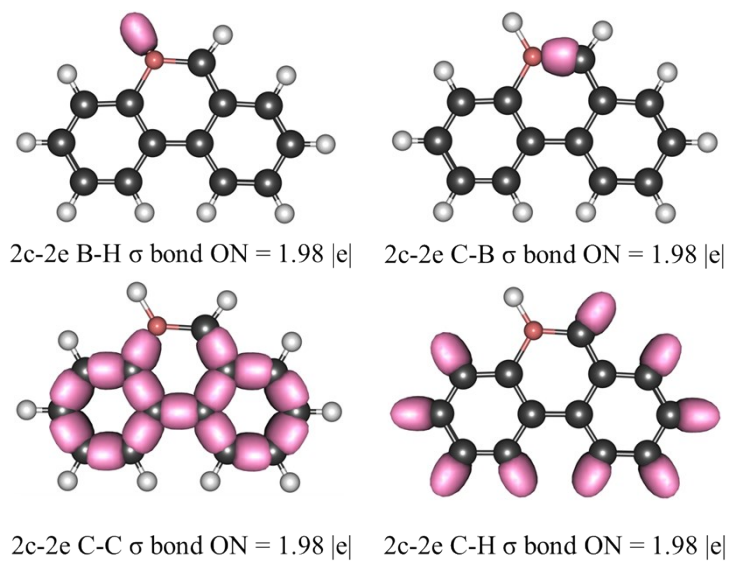


Table S1. Cartesian coordinates of the studied systems, computed at the B3LYP/6-311G** level of theory.

1				2			
C	-2.873756864	0.878907365	0.000006476	C	2.833761049	0.877269842	-0.000006625
C	-3.590266701	-0.302780155	-0.000002632	C	3.555703282	-0.296142359	0.000002517
C	-1.458560578	0.921414221	0.000006911	C	1.420998132	0.864850507	-0.000006696
C	-2.889690205	-1.521203416	-0.000011915	C	2.878005712	-1.527081142	0.000011955
C	-0.750340414	-0.325733711	-0.000002579	C	0.728321650	-0.379838696	0.000002868
C	-1.507763521	-1.524969931	-0.000011827	C	1.498344277	-1.564397753	0.000012098
B	-0.687136229	2.261100014	0.000017218	C	0.677931572	2.091356580	-0.000016336
C	0.783477218	2.171477042	0.000016687	C	-0.678556155	2.091482175	-0.000016174
C	1.443152873	0.912566441	0.000007120	C	-1.421122753	0.864785313	-0.000006737
C	0.712591570	-0.335441615	-0.000002519	C	-0.728190515	-0.379846974	0.000002757
H	-3.405001439	1.827980327	0.000013706	H	3.344748873	1.834528234	-0.000013963
H	-4.677293541	-0.295301240	-0.00002671	H	4.639470443	-0.272134471	0.000002443
H	-3.431380194	-2.463651772	-0.000019179	H	3.440772921	-2.453764090	0.000019196
H	-1.004686850	-2.485207992	-0.000019119	H	1.005882176	-2.528130607	0.000019501
H	-1.305709248	3.302308545	0.000025129	H	1.228668814	3.026045477	-0.000022272
H	1.446909598	3.039199045	0.000023399	H	-1.229381918	3.026199145	-0.000023054
C	2.869912338	0.832274446	0.000006658	C	-2.833751836	0.877076518	-0.000006700
C	1.452315551	-1.538785780	-0.000011661	C	-1.498071708	-1.564529740	0.000011835
C	2.835373521	-1.574646207	-0.000011785	C	-2.877741425	-1.527237371	0.000011624
C	3.551751614	-0.362562744	-0.000002419	C	-3.555595288	-0.296444157	0.000002282
H	3.421702553	1.769310323	0.000013904	H	-3.344861402	1.834265032	-0.000013992
H	0.924636974	-2.485906829	-0.000018959	H	-1.005553007	-2.528224504	0.000019216
H	3.358121748	-2.526442473	-0.000019029	H	-3.440581989	-2.453878635	0.000018750
H	4.639203140	-0.370883764	-0.000002364	H	-4.639380880	-0.272721998	0.000002161
3				4			
C	-0.719400748	1.276728089	0.000000000	C	-1.207401599	-0.697092022	0.000000000
C	0.676409690	1.218312763	0.000000000	C	-1.207401599	0.697092069	0.000000000
C	1.372452184	0.000000000	0.000000000	C	0.000000000	1.394186959	0.000000000
C	0.676409690	-1.218312763	0.000000000	C	1.207401599	0.697092022	0.000000000
C	-0.719400748	-1.276728089	0.000000000	C	1.207401599	-0.697092069	0.000000000
B	-1.528939094	0.000000000	0.000000000	C	0.000000000	-1.394186959	0.000000000
H	-1.163253378	2.277357578	0.000000000	H	-2.146630345	-1.239328042	0.000000000
H	1.267755820	2.139337509	0.000000000	H	-2.146630329	1.239328122	0.000000000
H	2.462034765	0.000000000	0.000000000	H	0.000000065	2.478697636	0.000000000
H	1.267755820	-2.139337509	0.000000000	H	2.146630345	1.239328042	0.000000000
H	-1.163253378	-2.277357578	0.000000000	H	2.146630329	-1.239328122	0.000000000
H	-2.745164570	0.000000000	0.000000000	H	-0.000000065	-2.478697636	0.000000000