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Supporting Information

Aromaticity and Extrusion of Benzenoids Linked to [*o*-COSAN]$^{-}$: Clar Has the Answer

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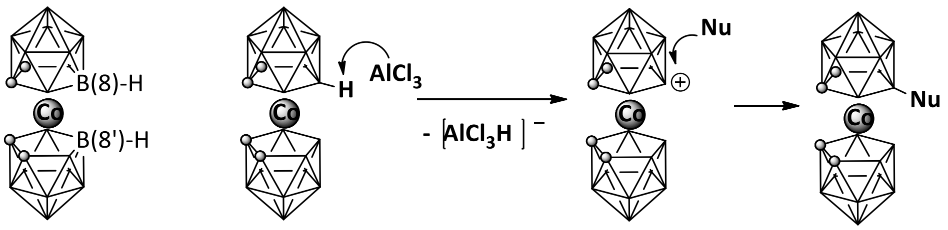
1.- General considerations:

The following reactions have been inspired in the Friedel-Craft reaction although no halogenated reagents, the typical R-Cl or RC(O)Cl leading to alkylation or acylation have not been used. In our case only B-H from $[3,3'\text{-}Co(1,2\text{-}C_2B_9H_{11})_2]^-$, $[\mathbf{1}]^-$ and double bonds from arenes have been the reacting sites used in mesitylene. Thus, these reactions have in common with the Friedel-Craft reaction the anhydrous $AlCl_3$.

Proposed reaction for the Cobaltabis(dicarbollide) arene coupling.

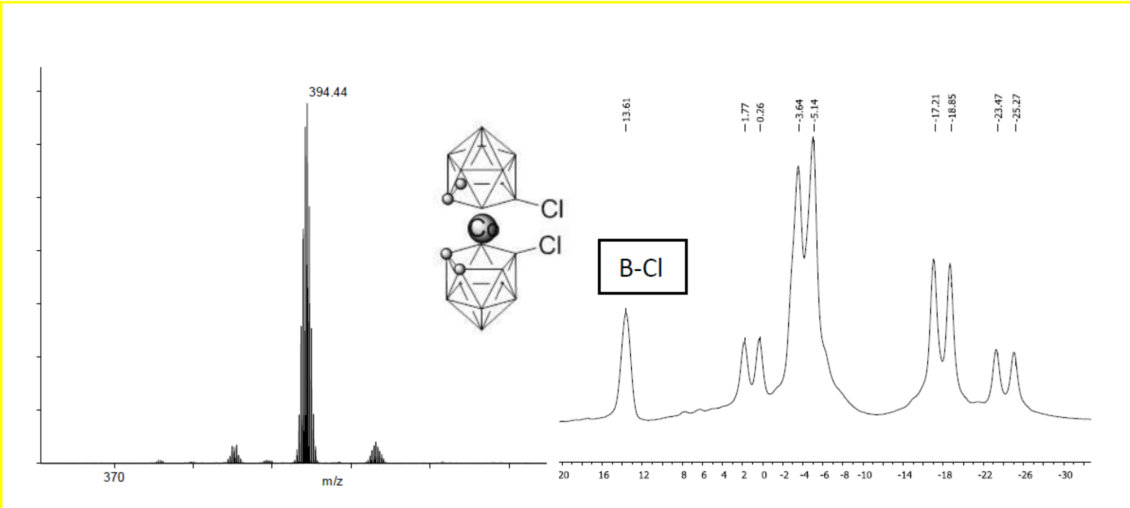
In a first step (Scheme S1), the Lewis acid removes the hydride of the B(8) vertex, the most electrophilic boron of the anionic $[3,3'\text{-}Co(1,2\text{-}C_2B_9H_{11})_2]^-$ cluster, and in a second step the nucleophilic attack by the aromatic substrate takes place.

Scheme S1: General pathway for the Electrophilic Induced Nucleophilic Substitution (EINS) reaction, which produces a B-C bond.



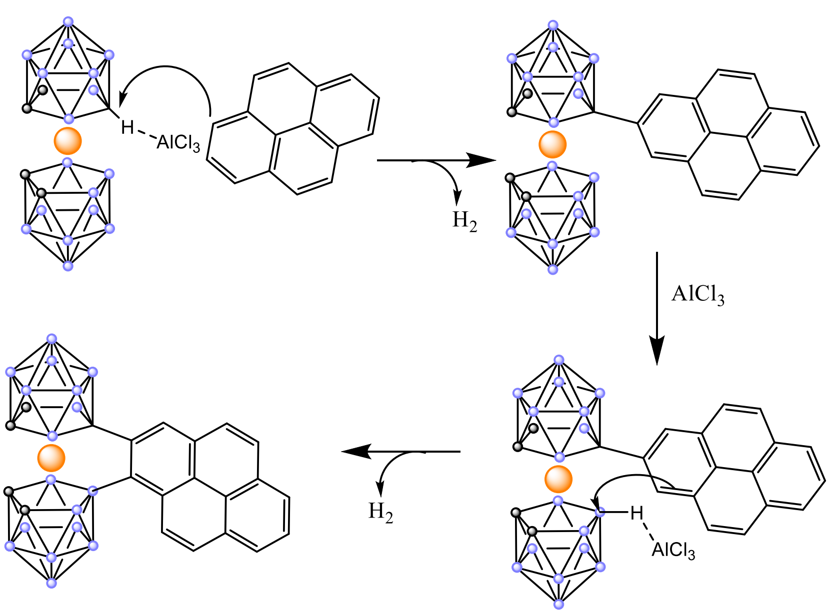
Unless otherwise noted, all manipulations were carried out under a dinitrogen atmosphere using standard vacuum line techniques. Dried anhydrous $AlCl_3$ was used as a catalyst, and the reactions were conducted in dried mesitylene. Minor amounts of water or just a bit of hydrated $AlCl_3$ or a slow T increase led to chlorinated $[3,3'\text{-}Co(1,2\text{-}C_2B_9H_{11})_2]^-$, which were unwanted byproducts, as confirmed by ^{11}B-NMR (the resonances of B-Cl vertices are found at downfield in the region near +15 ppm) and MALDI-TOF-MS spectra (Figure S1).

Figure S1. MALDI-TOF-MS (left) and ^{11}B-RMN spectra of $[3,3'-Co(8-Cl-1,2-C_2B_9H_{10})_2]^-$ (right).



In a second step (Scheme S2), after the substitution at the B(8) vertex, the B(8') of the second cluster's moiety is also able to react, and further reaction on this B(8') vertex can go on as displayed in Scheme S2 in the case of arene = pyrene.

Scheme S2: Proposed pathway of the reaction between the anionic $[3,3'-Co(1,2-C_2B_9H_{11})_2]^-$ cluster, $AlCl_3$ as Lewis acid and pyrene as the nucleophilic substrate in mesitylene.



The solvent for these coupling reactions between cobaltabis(dicarbollide) and arenes must follow some requirements, which are: i) it does not react as a reagent, ii) it must have a high boiling point, and iii) it must be a good solvent for the reagents. Mesytilene (1,3,5-trimethylbenzene) with a molecular formula C_9H_{12}, melting and boiling points −44.8 and 164.7 °C, respectively, was considered to be the best option as a solvent for running the coupling reactions.

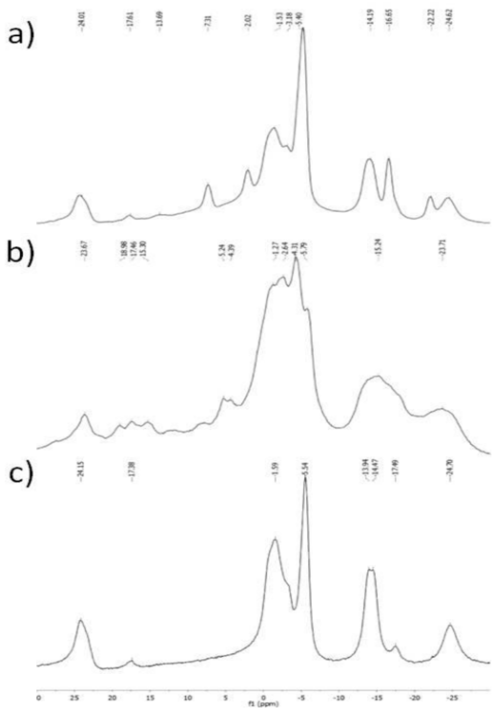
When studying the best conditions several Lewis acids, temperature and time of the reaction were tested. Lewis acids: $FeCl_3$, $AlCl_3$, $BF_3·Et_2O$ and $Sm(OTf)_3$ were tested, however, the best results were obtained with $AlCl_3$. The reaction was run at different temperatures but the best yields were achieved at 160 ºC (see Table S1). Reaction times studied were in the range 1 - 5h (see Table S1).

Table S1. The percentage of the different products that can be obtained by the reaction with pyrene with [**1**]$^-$ at different temperatures and times. % B-C(sp^3) refers to CH_2 extrusion. % B-C(sp^2) refers to non-extrusion. The (–) sign refers to undetected material most probably unreacted [**1**]$^-$. In blue, the optimal conditions found.

Time (hours)	**T (ºC)**	**% B-Cl**	**% B-C(sp^3)**	**% B-C(sp^2)**
1	r.t.	80	-	-
1	80	75	-	5
1	160	-	-	70
2	r.t.	100	0	0
2	80	60	0	40
2	**160**	**0**	**0**	**100**
5	r-t-	100	0	0
5	80	60	20	20
5	160	0	90	10

From Table S1, it is quite clear that for pyrene high temperature and relatively short reactions times (2h) leads to the non-extruded compounds. Extended reaction times leads to the extruded species. This, as is discussed in the paper, depends on the possibility to preserve the Clar's sextets. Figure S2 shows the influence of T and time on the evolution of the reaction. The $AlCl_3$ at low T becomes an undesirable chlorinating agent leading to the di-chlorinated [**1**]$^-$ cluster at the B(8) and B(8') vertices, as observed by ^{11}B-NMR spectrum (Figure S1-c) and supported by MALDI-TOF-MS spectrum (Figure S2 left).

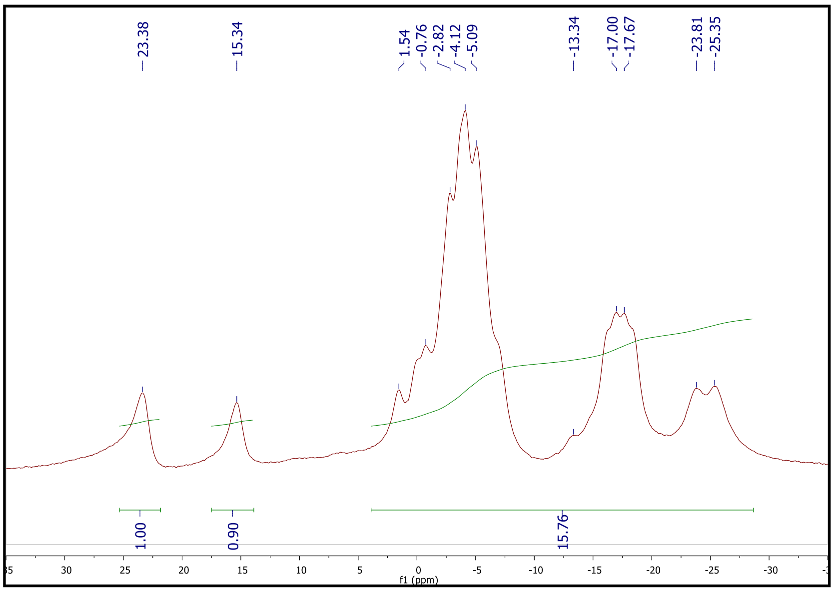
Figure S2. ^{11}B-RMN spectra of the reaction of pyrene and [**1**]$^-$ at different reaction conditions a) 160 ºC, 1 h, b) 80 ºC, 1 h and c) 160 ºC and 2 h.



2.- Representative ^{11}B-NMR spectra of an extruded (anthracene; Figure S3) and non-extruded (pyrene; Figure S4) arene coupling with cobaltabis(dicarbollide).

Figure S3. a) ^{11}B NMR and b) ^{11}B{^{1}H} NMR spectra of **extruded** [8,8'-μ-anthracenyl-3,3'-Co(1,2-$C_2B_9H_{10}$)$_2$]$^-$ displaying the two characteristic B-C(sp^2) and B-C(sp^3) resonances that are singlets in the ^{11}B NMR spectrum when any other resonances are a doublet, and the integration.

a)



b)

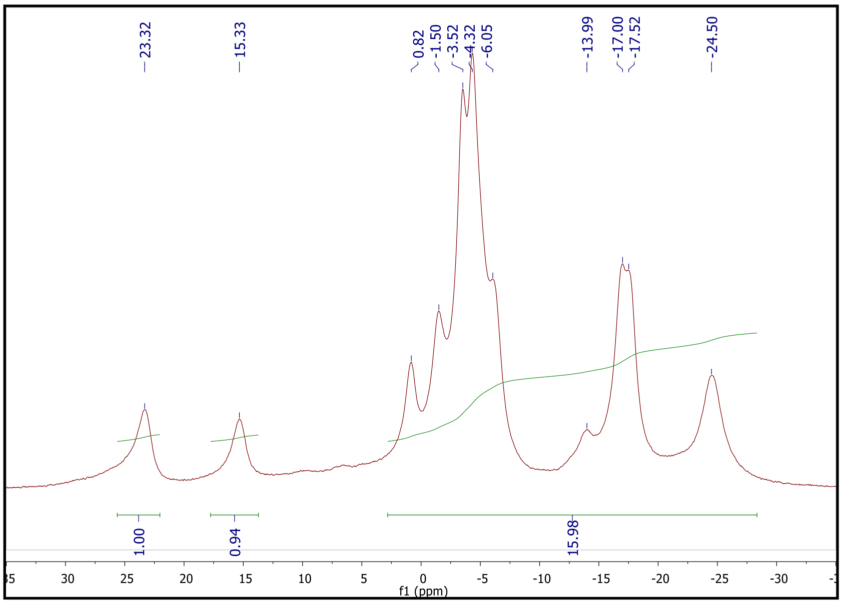
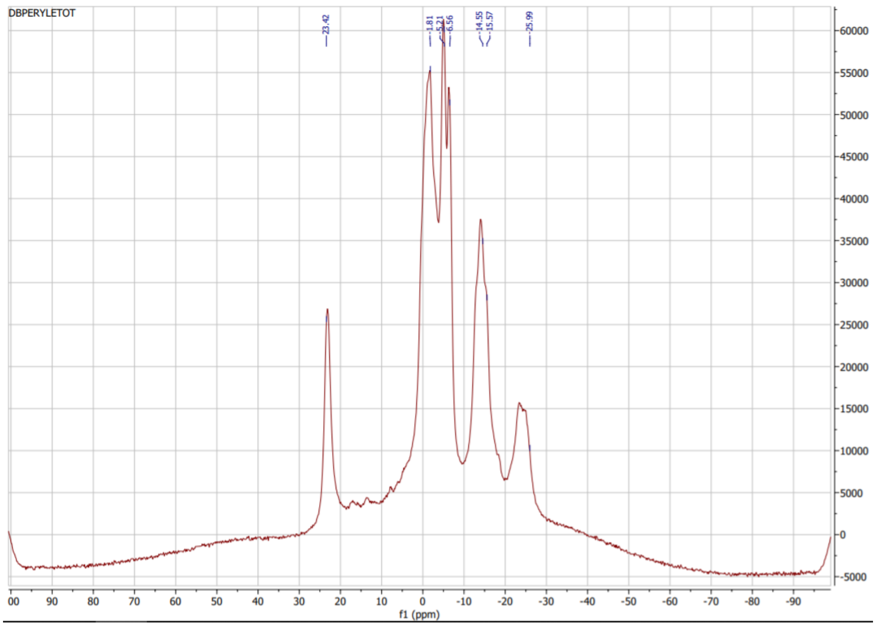


Figure S4. a) ^{11}B NMR and b) $^{11}B\{^1H\}$ NMR spectra of **non-extruded** [8,8'-μ-pyrene-3,3'-Co(1,2-$C_2B_9H_{10}$)$_2$]$^-$ displaying the characteristic B-C(sp^2) resonance that is a singlet in the ^{11}B NMR spectrum when any other resonances are a doublet, and the integration.

a)



b)

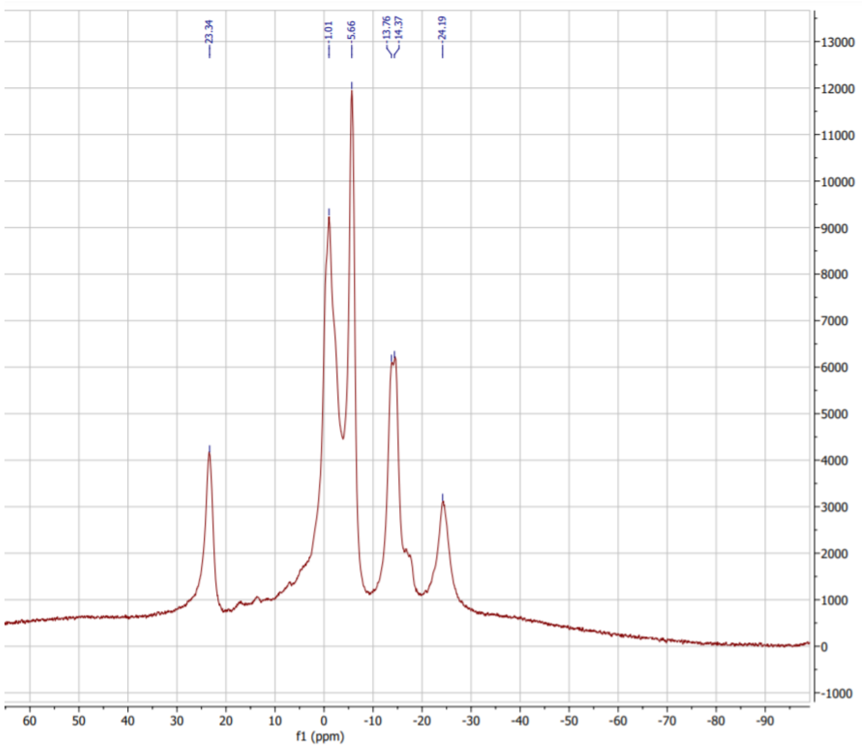


Figure S5 displays the $^{13}C\{^1H\}$ NMR of the **non-extruded** [8,8'-μ-pyrene-3,3'-Co(1,2-$C_2B_9H_{10})_2]^-$. The spectrum shows two different C_c-H resonances at 46.3 and 45.2 ppm, different from the ones of the parent starting Cs[3,3'-Co(1,2-$C_2B_9H_{11})_2$] cluster. These indicate that the two halves, the upper and the lower, are not equivalent proving that the pyrene is not symmetrically distributed, ruling out a fully symmetric pyrene as would be the structure in Chart 1 right.

Figure S5. $^{13}C\{^1H\}$ NMR of the **non-extruded** [8,8'-μ-pyrene-3,3'-Co(1,2-$C_2B_9H_{10})_2]^-$.

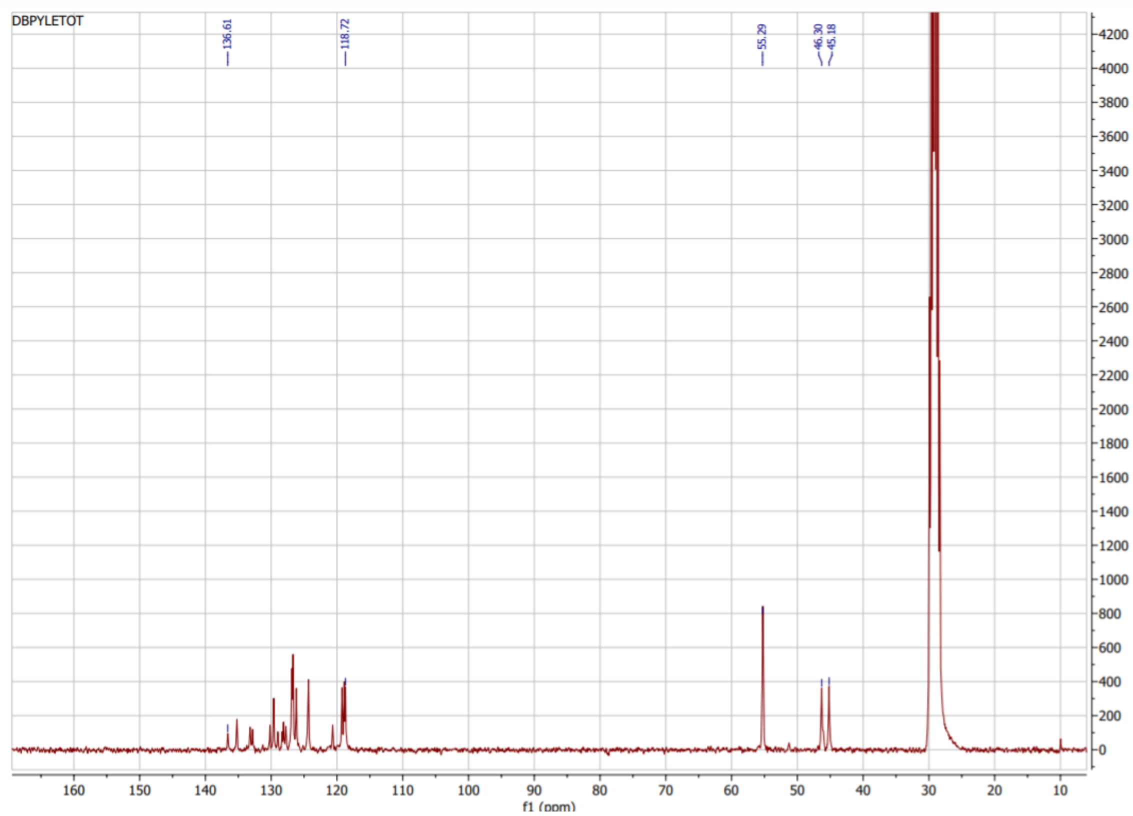
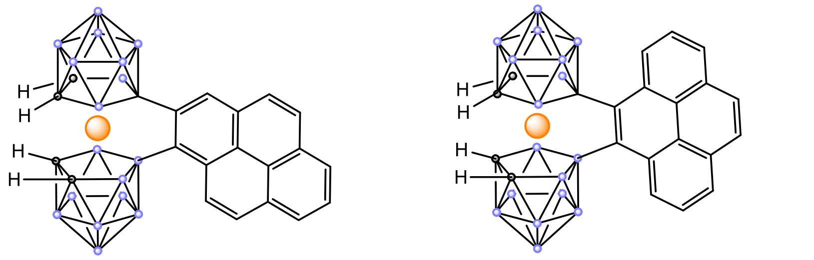


Chart 1. The two possible isomers of **non-extruded** [8,8'-μ-pyrene-3,3'-Co(1,2-$C_2B_9H_{10})_2]^-$. The one in b) has a higher symmetry than the one in a). In b) only one cluster C resonance would be observed, whereas two would be found in a).



a) Upper C distinct to lower C in metallacarborane

b) Upper C equivalent to lower C in metallacarborane

As the $^{13}C\{^1H\}$ NMR shows two ^{13}C resonances in the 46.3 and 45.2 ppm region, the ^{13}C-NMR proves that the **non-extruded** [8,8'-μ-pyrene-3,3'-Co(1,2-$C_2B_9H_{10})_2]^-$ is the one represented by a) at the Chart 1. The MALDI-TOF-MS spectrum shows a single peak with the corresponding isotopic distribution centered at 522 m/e.

3.- Synthesis of [NC_4H_{12}][8,8'-μ-arenyl-[3,3'-Co($C_2B_9H_{10})_2$], arene = Naphthalene, Anthracene, Pyrene, and Perylene.

General considerations: To run the NMR spectra it was attempted that the concentration of the complexes was near to 1×10^{-3} mol L^{-1}. ^1H and $^1H\{^{11}B\}$ NMR (300.13 MHz), $^{13}C\{^1H\}$ NMR (75.47 MHz), and ^{11}B and $^{11}B\{^1H\}$ NMR (96.29 MHz) spectra were recorded with a Bruker ARX 300 instrument equipped with the appropriate decoupling accessories. Chemical shift values for ^{11}B and $^{11}B\{^1H\}$ NMR spectra are referenced to external $BF_3{\cdot}OEt_2$, and those for ^1H, $^1H\{^{11}B\}$, and $^{13}C\{^1H\}$ NMR spectra are referenced to $SiMe_4$. Chemical shifts are reported in units of parts per million downfield from the reference signal, and all coupling constants are reported in Hertz. . The mass spectra were recorded in the negative ion mode using a Bruker Biflex MALDI-TOF-MS [N_2 laser; λexc 337 nm (0.5 ns pulses); voltage ion source 20.00 kV (Uis1) and 17.50 kV (Uis2)]. MALDI-TOF-MS spectra were run using Cs[3,3'-Co(1,2-$C_2B_9H_{11})_2$], [**1**]$^-$, as the reference with the base peak of the molecular ion set at 324 m/e. Unless otherwise noted, all manipulations were carried out under a dinitrogen atmosphere using standard vacuum line techniques. Dried anhydrous $AlCl_3$ was used as a catalyst, and the reactions were conducted in dried mesitylene. The cesium salt of compound [**1**]$^–$ was supplied by Katchem Ltd. (Prague) and was used as received. All other reagents were obtained commercially and were used as purchased.

General procedure: The Cs**[1]** (50 mg, 0.11 mmol) was set for 3 hours at vacuum at 80ºC to remove any residual moisture. The corresponding dried arene (0.22-0.27 mmol) and 8.8 mg dried anhydrous $AlCl_3$ were added. Then, 3mL of dried mesytilene were added as a solvent. The mixture was immersed in an oil bath (160 °C) for 2 h. Mesytilene was evaporated under vacuum and the residue was extracted three times with Et_2O:HCl_{aq} (0.1M) in a ratio of 5:10 mL. The organic layer was dried over $MgSO_4$, filtered, and evaporated under vacuum. The residue was dissolved in the minimum volume of EtOH and an aqueous solution containing an excess of [NMe_4]Cl was added, resulting in the formation of an orange precipitate. This was filtered off, washed and dried in vacuum.

Data for naphthalene: [NC_4H_{12}][8,8'-μ-$C_{10}H_8$-Co($C_2B_9H_{10}$)$_2$]: Yield: 46 mg (80%). The spectral data is consistent with those reported earlier in cyclohexane.[1]

Data for anthracene: [NC_4H_{12}][8,8'-μ-$C_{14}H_{10}$-Co($C_2B_9H_{10}$)$_2$]. Yield: 49 mg (77%). ^{11}B-NMR: δ = 23.4 (s, 1B), 15.3 (s, 1B), 1.01 (d, ^{1}J(B,H) = 130 Hz, 1B), -0.2 (d, ^{1}J(B,H) = 130 Hz, 1B), -3.8 (d, ^{1}J(B,H) = 130 Hz, 4B), -4.6 (d, ^{1}J(B,H) = 130 Hz, 4B), -16.3 (d, ^{1}J(B,H) = 140 Hz, 2B), -18.3 (d, ^{1}J(B,H) = 140 Hz, 2B), -24.6 (d, ^{1}J(B,H) = 150 Hz, 2B). ^{1}H-NMR: 7.80-7.30 (m, 6H, H_{aryl}), 3.86 (s, 2H, C_c-H), 3.83 (s, 2H, C_c-H), 3.45 (s, 12H, (N(CH_3)$_4$), 2.16 (s, 2H, CH_2), and 2.06 (s, 2H, CH_2). MALDI-TOF-MS 500 m/e.

Data for pyrene: [NC_4H_{12}][8,8'-μ-$C_{16}H_8$-Co($C_2B_9H_{10}$)$_2$]. Yield: 49 mg (75%). ^{13}C{^{1}H}-NMR: δ = 136.6-118.7 ($\mathbf{C_{16}}H_8$), 55.3 (N($\mathbf{C}H_3$)$_4$), 46.3 ($\mathbf{C_c}$-H), 45.2 ($\mathbf{C_c}$-H). ^{11}B-NMR: δ = 23.3 (s, 2B), -1.01 (d, ^{1}J(B,H) = 130 Hz, 6B), -5.66 (d, ^{1}J(B,H) = 130 Hz, 4B), -13.76 (d, ^{1}J(B,H) = 126 Hz, 2B), -14.37 (d, ^{1}J(B,H) = 145 Hz, 2B), -24.19 (d, ^{1}J(B,H) = 120 Hz, 2B). MALDI-TOF-MS 522 m/e.

Data for perylene: [NC_4H_{12}][8,8'-μ-$C_{20}H_{10}$-Co($C_2B_9H_{10}$)$_2$]. Yield: 49 mg (69%). ^{1}H{^{11}B}-NMR: δ = 8.72-7.37 (10H, $C_{20}\mathbf{H_{10}}$), 3.90 (2H, C_c-**H**), 3.83 (2H, C_c-**H**), 3.45 (12H, N(C$\mathbf{H}_3$)$_4$), 3.20-1.61 (br.s, B-H) ^{13}C{^{1}H}-NMR: δ = 136.57-118.68 ($\mathbf{C_{20}}H_{12}$), 55.25 (N($\mathbf{C}H_3)_4$), 46.26 ($\mathbf{C}_c$-H), 45.14 ($\mathbf{C}_c$-H). ^{11}B-NMR: δ = 23.27 (s, 2B), -1.05 (d, ^{1}J(B,H) = 134 Hz, 6B), -5.75 (d, ^{1}J(B,H) = 142 Hz, 4B), -14.09 (d, ^{1}J(B,H) = 145Hz, 2B), -14.40 (d, ^{1}J(B,H) = 151 Hz, 2B), -24.25 (d, ^{1}J(B,H) = 139 Hz, 2B). MALDI-TOF-MS 572 m/e.

Computational Details

Computational analysis: All calculations were performed with the Gaussian 09 package[2] by means of the B3LYP[3,4,5] hybrid density functional, with dispersion correction with Becke-Johnson damping, and the 6-311++G(d,p) basis set.[6] The geometry optimizations were carried out without symmetry constraints. Analytical Hessians were computed to characterize the optimized structures as minima (zero imaginary frequencies). Aromaticity was evaluated by means of the nucleus-independent chemical shift (NICS),[7,8,9,10] proposed by Schleyer and co-workers as a magnetic descriptor of aromaticity. NICS is defined as the negative value of the absolute shielding computed at a ring center or at some other point of the system. Rings with large negative NICS values are considered aromatic. NICS values were computed using the gauge-including atomic orbital method (GIAO).[11] Aromaticity of rings of benzenoids was further evaluated with the multicenter index (MCI),[12,13,14] which measures the electron sharing in the ring, and computed by means of ESI-3D software.[15,16,17,18] Thermodynamic data has also been computed at the BLYP-D3BJ/TZ2P//B3LYP(GD3BJ)/6-311++G** level by means of AMS software.[1918]

Table S2. Cartesian coordinates of fused systems between cosan and BENZENOIDs, with and without extrusion.

Benzene

1	5	0	3.052126	-2.299672	-0.000064
2	1	0	3.416424	-3.422828	-0.000178
3	5	0	3.938134	-0.777253	-0.000176
4	1	0	5.122971	-0.783894	-0.000393
5	5	0	3.006677	-1.271207	1.421182
6	1	0	3.425759	-1.692423	2.443763
7	5	0	1.468281	-0.358821	1.437402
8	1	0	1.063631	-0.183362	2.527224
9	5	0	3.006465	-1.271259	-1.421141
10	1	0	3.425058	-1.692915	-2.443754
11	5	0	1.468429	-0.358615	-1.437379
12	1	0	1.064255	-0.183078	-2.527380
13	5	0	2.961036	0.417982	-0.886847
14	1	0	3.467135	1.272645	-1.533959
15	5	0	2.960962	0.418128	0.886708

16	1	0	3.466691	1.273063	1.533743
17	5	0	1.425579	0.730750	-0.000036
18	1	0	-1.064530	-0.182765	2.527364
19	5	0	-1.468628	-0.358377	1.437328
20	5	0	-3.006650	-1.271004	1.421071
21	5	0	-2.961153	0.418169	0.886555
22	5	0	-1.425599	0.730820	-0.000121
23	1	0	-3.425371	-1.692466	2.443711
24	5	0	-3.052240	-2.299651	0.000137
25	5	0	-3.938148	-0.777147	-0.000051
26	1	0	-3.467316	1.272898	1.533530
27	5	0	-2.960853	0.418098	-0.886963
28	5	0	-1.468079	-0.358885	-1.437391
29	1	0	-3.416548	-3.422801	0.000302
30	5	0	-3.006487	-1.271317	-1.421217
31	1	0	-5.122986	-0.783697	-0.000028
32	1	0	-3.466528	1.272944	-1.534160
33	1	0	-1.063461	-0.183759	-2.527264
34	1	0	-3.425477	-1.692551	-2.443828
35	27	0	-0.000019	-0.838938	0.000132
36	6	0	-1.570449	-1.922411	0.799773
37	6	0	-1.570354	-1.922601	-0.799552
38	6	0	1.570401	-1.922507	0.799776
39	6	0	1.570282	-1.922498	-0.799619
40	1	0	1.170324	-2.792837	1.300402
41	1	0	1.170052	-2.792784	-1.300179
42	1	0	-1.170237	-2.792587	1.300538
43	1	0	-1.170154	-2.792956	-1.300031
44	6	0	1.389457	3.356877	0.000261
45	6	0	0.696992	4.568509	0.000206
46	6	0	0.706236	2.137000	0.000092
47	6	0	-0.696823	4.568546	-0.000148
48	6	0	-0.706189	2.137037	-0.000186
49	6	0	-1.389349	3.356948	-0.000285
50	1	0	-2.474851	3.359604	-0.000513
51	1	0	2.474960	3.359481	0.000500
52	1	0	1.242076	5.507619	0.000371
53	1	0	-1.241858	5.507683	-0.000247

Benzene-extrusion

1	5	0	1.938520	-3.151754	0.202723
2	1	0	1.852245	-4.325307	0.299322
3	5	0	3.337069	-2.082415	0.117186
4	1	0	4.432980	-2.531233	0.157501
5	5	0	2.284752	-2.064328	1.541928
6	1	0	2.515328	-2.529376	2.604497
7	5	0	1.202448	-0.639034	1.431924
8	1	0	0.864293	-0.215620	2.478672
9	5	0	2.293668	-2.302579	-1.297349
10	1	0	2.525325	-2.941823	-2.265423
11	5	0	1.210293	-0.881574	-1.427917
12	1	0	0.846528	-0.645634	-2.527885
13	5	0	2.884736	-0.687748	-0.897457
14	1	0	3.687648	-0.148478	-1.583296
15	5	0	2.884250	-0.540817	0.876924
16	1	0	3.679850	0.111977	1.465394
17	5	0	1.587857	0.267505	-0.080647
18	1	0	-1.559825	-0.865969	2.477156
19	5	0	-1.852683	-0.431466	1.416538
20	5	0	-3.536037	-0.782963	0.914381

21	5	0	-3.012921	0.879537	1.194882
22	5	0	-1.316178	1.102931	0.629681
23	1	0	-4.218716	-1.460326	1.603490
24	5	0	-3.559550	-1.070127	-0.821746
25	5	0	-4.063629	0.495763	-0.193163
26	1	0	-3.419691	1.503948	2.118523
27	5	0	-2.699520	1.619117	-0.396072
28	5	0	-1.342804	0.764426	-1.144969
29	1	0	-4.163265	-1.940320	-1.343749
30	5	0	-3.032665	0.399621	-1.631078
31	1	0	-5.198792	0.828449	-0.262844
32	1	0	-2.878994	2.772332	-0.607223
33	1	0	-0.690320	1.246579	-1.998958
34	1	0	-3.358548	0.576018	-2.754043
35	27	0	-0.325373	-0.681442	-0.008298
36	6	0	-2.205420	-1.489020	0.145093
37	6	0	-1.919356	-0.819218	-1.290108
38	6	0	0.715728	-2.177750	0.929339
39	6	0	0.724541	-2.317550	-0.674769
40	1	0	0.006947	-2.778172	1.480921
41	1	0	0.019331	-3.007606	-1.117364
42	1	0	-2.099262	-2.562654	0.221469
43	1	0	-1.631718	-1.474995	-2.098597
44	6	0	1.625546	1.822250	-0.131404
45	6	0	2.697549	2.653789	-0.800147
46	6	0	-0.447556	2.273947	1.286330
47	6	0	2.317139	4.073825	-0.481660
48	6	0	0.762062	2.669359	0.490180
49	6	0	1.196485	4.055295	0.268195
50	1	0	0.669301	4.921682	0.653223
51	1	0	2.857759	4.947872	-0.822036
52	1	0	-0.131312	1.962124	2.290561
53	1	0	-1.086579	3.151439	1.434434
54	1	0	2.730543	2.467960	-1.882241
55	1	0	3.695684	2.396034	-0.422595

Naphthalene

1	5	0	-3.052316	-3.049008	0.000315
2	1	0	-4.175626	-3.412278	0.000541
3	5	0	-1.531392	-3.938897	0.000001
4	1	0	-1.539947	-5.123487	-0.000045
5	5	0	-2.022605	-3.006174	1.421304
6	1	0	-2.444227	-3.423854	2.444066
7	5	0	-1.109002	-1.468674	1.437197
8	1	0	-0.931216	-1.064503	2.526712
9	5	0	-2.023135	-3.006095	-1.421053
10	1	0	-2.445205	-3.423698	-2.443663
11	5	0	-1.109540	-1.468606	-1.437234
12	1	0	-0.932354	-1.064475	-2.526855
13	5	0	-0.334505	-2.963747	-0.886773
14	1	0	0.520105	-3.468814	-1.534385
15	5	0	-0.334175	-2.963811	0.886349
16	1	0	0.520735	-3.468859	1.533574
17	5	0	-0.022356	-1.428989	-0.000201
18	1	0	-0.932182	1.064601	2.526855
19	5	0	-1.109456	1.468722	1.437235
20	5	0	-2.023049	3.006201	1.421010
21	5	0	-0.334457	2.963818	0.886605
22	5	0	-0.022359	1.428988	0.000130
23	1	0	-2.445050	3.423887	2.443615

24	5	0	-3.052341	3.048996	-0.000292
25	5	0	-1.531417	3.938888	-0.000153
26	1	0	0.520190	3.468950	1.534116
27	5	0	-0.334264	2.963734	-0.886514
28	5	0	-1.109102	1.468548	-1.437198
29	1	0	-4.175652	3.412259	-0.000472
30	5	0	-2.022732	3.006043	-1.421343
31	1	0	-1.539974	5.123477	-0.000215
32	1	0	0.520596	3.468742	-1.533839
33	1	0	-0.931418	1.064373	-2.526720
34	1	0	-2.444414	3.423632	-2.444118
35	27	0	-1.587379	0.000005	0.000100
36	6	0	-2.673308	1.569189	0.799963
37	6	0	-2.673094	1.569077	-0.800309
38	6	0	-2.673023	-1.569160	0.800421
39	6	0	-2.673346	-1.569135	-0.799853
40	1	0	-3.542864	-1.168094	1.300978
41	1	0	-3.543388	-1.168015	-1.300011
42	1	0	-3.543305	1.168100	1.300226
43	1	0	-3.542967	1.167958	-1.300765
44	6	0	2.585562	-1.396117	-0.000349
45	6	0	3.830693	-0.715021	-0.000181
46	6	0	1.387335	-0.717798	-0.000206
47	6	0	5.073609	-1.397398	-0.000318
48	6	0	3.830690	0.715035	0.000153
49	6	0	1.387334	0.717803	0.000131
50	6	0	6.264444	-0.707170	-0.000143
51	1	0	5.068224	-2.482944	-0.000563
52	6	0	5.073605	1.397415	0.000330
53	6	0	2.585557	1.396126	0.000290
54	6	0	6.264442	0.707191	0.000196
55	1	0	7.206429	-1.245234	-0.000253
56	1	0	5.068216	2.482961	0.000577
57	1	0	2.593057	2.482280	0.000507
58	1	0	7.206425	1.245258	0.000340
59	1	0	2.593066	-2.482271	-0.000565

Naphthalene-extrusion

1	5	0	2.914524	3.030963	0.250452
2	1	0	4.036465	3.386787	0.340843
3	5	0	1.400437	3.930718	0.206031
4	1	0	1.408680	5.113189	0.276611
5	5	0	1.794430	2.910736	1.601003
6	1	0	2.152108	3.271256	2.668634
7	5	0	0.876291	1.377335	1.463332
8	1	0	0.625242	0.881520	2.502352
9	5	0	1.976605	3.079394	-1.237932
10	1	0	2.470696	3.556816	-2.200684
11	5	0	1.060696	1.549078	-1.395253
12	1	0	0.961539	1.152815	-2.504716
13	5	0	0.263026	3.017299	-0.817666
14	1	0	-0.545378	3.576371	-1.480352
15	5	0	0.147797	2.915029	0.956340
16	1	0	-0.748092	3.392269	1.568419
17	5	0	-0.126409	1.437132	-0.034613
18	1	0	2.137010	-1.118527	2.429119
19	5	0	1.821766	-1.529773	1.365749
20	5	0	2.756807	-2.953189	0.810617
21	5	0	1.024027	-3.082706	1.121349
22	5	0	0.185228	-1.573717	0.606485

23	1	0	3.650581	-3.355091	1.473155
24	5	0	2.998646	-2.827749	-0.928970
25	5	0	1.738976	-3.886350	-0.299746
26	1	0	0.608435	-3.709729	2.038908
27	5	0	0.189308	-3.026548	-0.452450
28	5	0	0.471466	-1.434282	-1.169796
29	1	0	4.018838	-3.058305	-1.476496
30	5	0	1.421810	-2.859112	-1.708168
31	1	0	1.844118	-5.062200	-0.398611
32	1	0	-0.821326	-3.611876	-0.655971
33	1	0	-0.232712	-0.983310	-1.999035
34	1	0	1.355286	-3.199790	-2.838276
35	27	0	1.463939	0.013021	-0.018930
36	6	0	2.911007	-1.438103	0.073182
37	6	0	2.155863	-1.384507	-1.346873
38	6	0	2.478750	1.514546	0.943262
39	6	0	2.582788	1.613453	-0.657817
40	1	0	3.305754	1.065764	1.474071
41	1	0	3.481583	1.229901	-1.121049
42	1	0	3.871150	-0.945248	0.143161
43	1	0	2.643897	-0.858329	-2.154115
44	6	0	-1.588003	0.894336	-0.080358
45	6	0	-2.745179	1.606161	-0.754951
46	6	0	-1.206844	-1.209243	1.304538
47	6	0	-3.933543	0.732125	-0.450781
48	6	0	-2.041370	-0.230379	0.533675
49	6	0	-3.488615	-0.358159	0.327049
50	6	0	-4.396551	-1.328313	0.753773
51	6	0	-5.266807	0.852130	-0.805077
52	1	0	-1.012589	-0.805431	2.306215
53	1	0	-1.774737	-2.131769	1.460782
54	1	0	-2.574554	1.709266	-1.833752
55	1	0	-2.870428	2.624719	-0.368437
56	1	0	-4.064439	-2.170063	1.350968
57	6	0	-5.741211	-1.201800	0.396346
58	6	0	-6.177341	-0.123967	-0.376532
59	1	0	-5.607744	1.689832	-1.406129
60	1	0	-7.224946	-0.041953	-0.645867
61	1	0	-6.455594	-1.951420	0.720931

Anthracene

1	5	0	-3.901610	-3.048322	-0.000203
2	1	0	-5.024906	-3.411245	-0.000258
3	5	0	-2.381163	-3.939343	-0.000236
4	1	0	-2.390163	-5.123781	-0.000346
5	5	0	-2.871813	-3.006383	1.421026
6	1	0	-3.293348	-3.423539	2.443882
7	5	0	-1.958254	-1.468934	1.437183
8	1	0	-1.779703	-1.064812	2.526518
9	5	0	-2.871724	-3.006055	-1.421363
10	1	0	-3.293230	-3.423037	-2.444304
11	5	0	-1.958101	-1.468683	-1.437163
12	1	0	-1.779649	-1.064470	-2.526476
13	5	0	-1.183586	-2.964878	-0.886596
14	1	0	-0.328689	-3.469301	-1.534161
15	5	0	-1.183628	-2.965049	0.886340
16	1	0	-0.328746	-3.469555	1.533861
17	5	0	-0.872319	-1.430436	0.000027
18	1	0	-1.779266	1.064585	2.526433
19	5	0	-1.957904	1.468793	1.437141

20	5	0	-2.871501	3.006172	1.421377
21	5	0	-1.183448	2.964937	0.886348
22	5	0	-0.872320	1.430426	-0.000216
23	1	0	-3.292848	3.423228	2.444354
24	5	0	-3.901612	3.048337	0.000371
25	5	0	-2.381158	3.939339	0.000101
26	1	0	-0.328456	3.469409	1.533748
27	5	0	-1.183769	2.964965	-0.886589
28	5	0	-1.958463	1.468812	-1.437208
29	1	0	-5.024910	3.411256	0.000552
30	5	0	-2.872041	3.006261	-1.421005
31	1	0	-2.390153	5.123777	0.000092
32	1	0	-0.328990	3.469433	-1.534277
33	1	0	-1.780134	1.064685	-2.526569
34	1	0	-3.293718	3.423323	-2.443842
35	27	0	-2.435359	0.000007	0.000103
36	6	0	-3.521917	1.569010	0.800437
37	6	0	-3.522201	1.569029	-0.799857
38	6	0	-3.522072	-1.569094	0.800086
39	6	0	-3.522021	-1.568946	-0.800218
40	1	0	-4.391831	-1.167869	1.300603
41	1	0	-4.391710	-1.167620	-1.300769
42	1	0	-4.391527	1.167729	1.301161
43	1	0	-4.392038	1.167770	-1.300210
44	6	0	1.729393	-1.400894	0.000192
45	6	0	2.984740	-0.721344	0.000086
46	6	0	0.538706	-0.723144	0.000033
47	6	0	4.205828	-1.400000	0.000270
48	6	0	2.984738	0.721342	-0.000217
49	6	0	0.538705	0.723135	-0.000246
50	6	0	5.429521	-0.721205	0.000184
51	1	0	4.203635	-2.486023	0.000490
52	6	0	4.205824	1.400007	-0.000328
53	6	0	1.729391	1.400888	-0.000380
54	6	0	5.429516	0.721220	-0.000143
55	1	0	1.736934	-2.486810	0.000388
56	1	0	4.203622	2.486030	-0.000556
57	1	0	1.736927	2.486805	-0.000584
58	1	0	8.809302	1.246513	-0.000230
59	1	0	8.809304	-1.246513	0.000351
60	6	0	6.683464	-1.401932	0.000370
61	6	0	7.865800	-0.711855	0.000209
62	6	0	7.865799	0.711853	-0.000117
63	6	0	6.683471	1.401937	-0.000266
64	1	0	6.680479	2.487262	-0.000511
65	1	0	6.680460	-2.487257	0.000648

Anthracene-extrusion

1	5	0	4.022397	-2.742673	-0.334437
2	1	0	5.174332	-2.977264	-0.439877
3	5	0	2.609815	-3.795385	-0.308793
4	1	0	2.739659	-4.968147	-0.412114
5	5	0	2.886223	-2.703644	-1.677869
6	1	0	3.272458	-2.996093	-2.756088
7	5	0	1.814066	-1.279293	-1.496376
8	1	0	1.504753	-0.784765	-2.520232
9	5	0	3.103698	-2.928538	1.155228
10	1	0	3.651124	-3.377061	2.102662
11	5	0	2.034093	-1.506406	1.357519
12	1	0	1.901494	-1.151673	2.477424

13	5	0	1.390350	-3.033606	0.742928
14	1	0	0.649419	-3.692214	1.392643
15	5	0	1.253229	-2.896895	-1.026529
16	1	0	0.408321	-3.449139	-1.647876
17	5	0	0.837258	-1.480957	0.005231
18	1	0	2.798320	1.359599	-2.401159
19	5	0	2.449358	1.705950	-1.325261
20	5	0	3.236271	3.201778	-0.736107
21	5	0	1.496292	3.161327	-1.036208
22	5	0	0.823761	1.559111	-0.557515
23	1	0	4.078212	3.711002	-1.392395
24	5	0	3.502867	3.058777	0.998150
25	5	0	2.135141	3.997221	0.402543
26	1	0	1.012046	3.765963	-1.934771
27	5	0	0.684369	2.977200	0.539002
28	5	0	1.136984	1.405254	1.212928
29	1	0	4.497747	3.379672	1.546442
30	5	0	1.936707	2.906844	1.785454
31	1	0	2.118254	5.174457	0.532311
32	1	0	-0.380904	3.445966	0.764031
33	1	0	0.488065	0.862702	2.032251
34	1	0	1.842277	3.208619	2.924440
35	27	0	2.266250	0.099384	0.019502
36	6	0	3.552485	1.693760	-0.040187
37	6	0	2.817164	1.526010	1.382328
38	6	0	3.425996	-1.262653	-0.983905
39	6	0	3.550015	-1.392356	0.612942
40	1	0	4.197406	-0.715185	-1.504823
41	1	0	4.404315	-0.925770	1.084113
42	1	0	4.558627	1.306695	-0.126931
43	1	0	3.362166	1.028879	2.171395
44	6	0	-0.674052	-1.100752	0.072717
45	6	0	-1.735589	-1.959778	0.733175
46	6	0	-0.527169	1.064830	-1.257718
47	6	0	-3.018899	-1.220906	0.454240
48	6	0	-1.249684	-0.015519	-0.509813
49	6	0	-2.699040	-0.049384	-0.303965
50	6	0	-3.695816	0.811739	-0.705622
51	6	0	-4.308592	-1.509492	0.796000
52	1	0	-0.297075	0.706173	-2.269040
53	1	0	-1.190812	1.925033	-1.389370
54	1	0	-1.546609	-2.069909	1.807900
55	1	0	-1.746534	-2.975527	0.320713
56	1	0	-3.465857	1.702945	-1.279466
57	6	0	-5.047020	0.536386	-0.367772
58	6	0	-5.363084	-0.639131	0.393015
59	1	0	-4.552618	-2.398314	1.371095
60	6	0	-6.716333	-0.899135	0.717333
61	6	0	-6.110505	1.390065	-0.761105
62	1	0	-5.872461	2.279882	-1.335089
63	6	0	-7.415842	1.108162	-0.429361
64	6	0	-7.724713	-0.049931	0.318867
65	1	0	-6.948291	-1.790266	1.292477
66	1	0	-8.755146	-0.267068	0.577807
67	1	0	-8.211751	1.775639	-0.741470

Phenanthrene

1	5	0	3.044043	3.533405	0.000311
2	1	0	4.057740	4.138162	0.000496
3	5	0	1.361936	4.062405	-0.000022

4	1	0	1.106369	5.219006	-0.000104
5	5	0	2.047769	3.263761	1.421241
6	1	0	2.365549	3.765227	2.443706
7	5	0	1.498922	1.562320	1.437635
8	1	0	1.415132	1.127643	2.526590
9	5	0	2.048307	3.263687	-1.420983
10	1	0	2.366496	3.765106	-2.443345
11	5	0	1.499483	1.562235	-1.437526
12	1	0	1.416208	1.127584	-2.526528
13	5	0	0.411774	2.846410	-0.886095
14	1	0	-0.534308	3.148436	-1.533213
15	5	0	0.411442	2.846466	0.885727
16	1	0	-0.534901	3.148494	1.532459
17	5	0	0.450295	1.280451	-0.000128
18	1	0	1.887840	-0.946863	2.526353
19	5	0	2.150560	-1.303095	1.437318
20	5	0	3.381675	-2.599524	1.421333
21	5	0	1.726253	-2.931589	0.886330
22	5	0	1.082781	-1.504644	0.000371
23	1	0	3.885567	-2.913318	2.443853
24	5	0	4.395918	-2.411646	0.000136
25	5	0	3.109406	-3.616353	0.000312
26	1	0	1.003935	-3.612692	1.533774
27	5	0	1.726122	-2.931675	-0.885530
28	5	0	2.150300	-1.303227	-1.436752
29	1	0	5.571602	-2.517385	0.000036
30	5	0	3.381438	-2.599654	-1.420860
31	1	0	3.379820	-4.769580	0.000340
32	1	0	1.003668	-3.612814	-1.532784
33	1	0	1.887297	-0.947172	-2.525767
34	1	0	3.885125	-2.913548	-2.443449
35	27	0	2.292186	0.236389	0.000240
36	6	0	3.698411	-1.052811	0.800561
37	6	0	3.698257	-1.052877	-0.800310
38	6	0	3.002798	2.007065	0.801405
39	6	0	3.003119	2.007031	-0.800716
40	1	0	3.939701	1.807635	1.301920
41	1	0	3.940227	1.807587	-1.300839
42	1	0	4.457126	-0.468717	1.301901
43	1	0	4.456880	-0.468832	-1.301843
44	6	0	-2.089013	0.670280	-0.000362
45	6	0	-3.155751	-0.255240	-0.000274
46	6	0	-0.764274	0.270671	-0.000122
47	1	0	-6.579120	2.892407	-0.001455
48	6	0	-2.832969	-1.640717	0.000089
49	6	0	-0.446977	-1.118932	0.000246
50	1	0	-8.342803	1.129914	-0.001106
51	1	0	-2.301261	1.731971	-0.000608
52	6	0	-3.884636	-2.611647	0.000205
53	6	0	-1.477353	-2.038388	0.000343
54	6	0	-5.193007	-2.243372	0.000003
55	1	0	-5.979776	-2.990968	0.000107
56	1	0	-3.608523	-3.661247	0.000468
57	1	0	-1.253151	-3.101090	0.000609
58	6	0	-5.566959	-0.860993	-0.000365
59	6	0	-4.553078	0.141967	-0.000526
60	6	0	-4.963750	1.494017	-0.000935
61	6	0	-6.299175	1.844741	-0.001140
62	6	0	-7.294717	0.851636	-0.000954
63	6	0	-6.926385	-0.477071	-0.000579

64	1	0	-7.683501	-1.255088	-0.000447
65	1	0	-4.217321	2.276826	-0.001092

Phenanthrene-extrusion

1	5	0	-3.342857	3.269163	-0.205086
2	1	0	-4.424087	3.742725	-0.203469
3	5	0	-1.745297	3.996121	-0.353842
4	1	0	-1.633859	5.168423	-0.481674
5	5	0	-2.386885	2.974523	-1.652422
6	1	0	-2.812105	3.330789	-2.696302
7	5	0	-1.627204	1.355359	-1.530705
8	1	0	-1.538515	0.795843	-2.564122
9	5	0	-2.255896	3.270910	1.179607
10	1	0	-2.594992	3.836578	2.161241
11	5	0	-1.497667	1.654000	1.321681
12	1	0	-1.327437	1.292539	2.434218
13	5	0	-0.611977	3.001797	0.595872
14	1	0	0.315250	3.492926	1.147547
15	5	0	-0.692078	2.820761	-1.172924
16	1	0	0.182535	3.171436	-1.891944
17	5	0	-0.479060	1.359618	-0.141859
18	1	0	-3.234700	-1.020437	-2.243061
19	5	0	-2.859386	-1.422965	-1.195873
20	5	0	-3.883869	-2.707222	-0.484946
21	5	0	-2.216072	-3.047981	-0.955657
22	5	0	-1.168272	-1.625179	-0.596877
23	1	0	-4.878430	-3.029233	-1.038395
24	5	0	-3.934029	-2.493019	1.261552
25	5	0	-2.868197	-3.710910	0.565546
26	1	0	-1.967649	-3.753131	-1.877031
27	5	0	-1.227631	-3.026475	0.526174
28	5	0	-1.261282	-1.387161	1.190389
29	1	0	-4.913027	-2.584481	1.914766
30	5	0	-2.299848	-2.674797	1.886069
31	1	0	-3.090532	-4.862613	0.730936
32	1	0	-0.270368	-3.712981	0.661691
33	1	0	-0.430476	-0.988943	1.923802
34	1	0	-2.155768	-2.977903	3.019539
35	27	0	-2.200811	0.121404	0.068327
36	6	0	-3.796000	-1.159357	0.190112
37	6	0	-2.899612	-1.139734	1.526369
38	6	0	-3.143409	1.689327	-0.862830
39	6	0	-3.072073	1.860008	0.734703
40	1	0	-4.063595	1.315116	-1.286841
41	1	0	-3.954372	1.595912	1.301242
42	1	0	-4.699707	-0.565394	0.189146
43	1	0	-3.241789	-0.532243	2.351455
44	6	0	0.912807	0.662174	-0.203919
45	6	0	2.198992	1.266524	0.324215
46	6	0	0.183858	-1.446365	-1.433321
47	6	0	3.247818	0.248799	-0.030310
48	6	0	1.185865	-0.533153	-0.791095
49	6	0	2.625253	-0.805410	-0.694294
50	6	0	3.382483	-1.911439	-1.144894
51	6	0	4.635015	0.247684	0.214972
52	1	0	-0.060603	-1.067444	-2.433485
53	1	0	0.632234	-2.432391	-1.591433
54	1	0	2.138552	1.442559	1.405244
55	1	0	2.395721	2.244418	-0.131669
56	1	0	2.894305	-2.731801	-1.658568

57	6	0	4.739948	-1.938788	-0.921550
58	6	0	5.401170	-0.878432	-0.245872
59	6	0	5.312357	1.299577	0.890841
60	6	0	6.799033	-0.894541	-0.008745
61	1	0	5.332374	-2.782939	-1.260558
62	1	0	4.737264	2.149699	1.239733
63	6	0	6.668887	1.248335	1.102052
64	6	0	7.423849	0.139657	0.648012
65	1	0	7.373997	-1.746910	-0.357577
66	1	0	7.167820	2.060494	1.619752
67	1	0	8.493957	0.109590	0.820834

Pyrene

1	5	0	3.469589	-3.228075	0.000000
2	1	0	4.057384	-4.251502	0.000000
3	5	0	4.025338	-1.557407	0.000000
4	1	0	5.185062	-1.317481	0.000000
5	5	0	3.212085	-2.227643	1.420358
6	1	0	3.708252	-2.550147	2.443736
7	5	0	1.521624	-1.638895	1.434673
8	1	0	1.090451	-1.548566	2.524320
9	5	0	3.212085	-2.227643	-1.420358
10	1	0	3.708252	-2.550147	-2.443736
11	5	0	1.521624	-1.638895	-1.434673
12	1	0	1.090451	-1.548566	-2.524320
13	5	0	2.828619	-0.586299	-0.887876
14	1	0	3.166624	0.333100	-1.551813
15	5	0	2.828619	-0.586299	0.887876
16	1	0	3.166624	0.333100	1.551813
17	5	0	1.253635	-0.564873	0.000000
18	1	0	-0.977693	-2.035614	2.529764
19	5	0	-1.335288	-2.295782	1.440695
20	5	0	-2.636028	-3.520975	1.421321
21	5	0	-2.957534	-1.864300	0.885935
22	5	0	-1.520314	-1.231173	0.000000
23	1	0	-2.952040	-4.024391	2.443244
24	5	0	-2.449522	-4.534948	0.000000
25	5	0	-3.649896	-3.243038	0.000000
26	1	0	-3.635742	-1.137567	1.531147
27	5	0	-2.957534	-1.864300	-0.885935
28	5	0	-1.335288	-2.295782	-1.440695
29	1	0	-2.558368	-5.710261	0.000000
30	5	0	-2.636028	-3.520975	-1.421321
31	1	0	-4.804561	-3.506760	0.000000
32	1	0	-3.635742	-1.137567	-1.531147
33	1	0	-0.977693	-2.035614	-2.529764
34	1	0	-2.952040	-4.024391	-2.443244
35	27	0	0.198474	-2.431099	0.000000
36	6	0	-1.089869	-3.841276	0.800808
37	6	0	-1.089869	-3.841276	-0.800808
38	6	0	1.945665	-3.159225	0.801614
39	6	0	1.945665	-3.159225	-0.801614
40	1	0	1.728946	-4.091160	1.304058
41	1	0	1.728946	-4.091160	-1.304058
42	1	0	-0.507119	-4.601985	1.300411
43	1	0	-0.507119	-4.601985	-1.300411
44	6	0	0.562622	2.039917	0.000000
45	6	0	-0.467562	3.036869	0.000000
46	6	0	0.225348	0.661025	0.000000
47	1	0	2.550639	6.533048	0.000000

48	6	0	-1.833420	2.641402	0.000000
49	6	0	-1.143993	0.299777	0.000000
50	1	0	0.741122	8.224729	0.000000
51	6	0	1.919883	2.515875	0.000000
52	6	0	-2.854710	3.646508	0.000000
53	6	0	-2.135554	1.276325	0.000000
54	6	0	-2.548641	4.970967	0.000000
55	1	0	-3.333238	5.720826	0.000000
56	1	0	-3.889876	3.320347	0.000000
57	1	0	-3.178363	0.975005	0.000000
58	6	0	-1.183827	5.410634	0.000000
59	6	0	-0.146821	4.427606	0.000000
60	6	0	1.215165	4.848779	0.000000
61	6	0	1.511800	6.219711	0.000000
62	6	0	0.493694	7.168496	0.000000
63	6	0	-0.839667	6.771096	0.000000
64	1	0	-1.631170	7.513456	0.000000
65	6	0	2.229628	3.839407	0.000000
66	1	0	3.268998	4.152302	0.000000
67	1	0	2.718076	1.794771	0.000000

Pyrene-extrusion

1	5	0	-3.479206	3.201928	-0.318153
2	1	0	-4.559542	3.675501	-0.278179
3	5	0	-1.896248	3.917389	-0.611013
4	1	0	-1.795038	5.079224	-0.817187
5	5	0	-2.611451	2.818398	-1.799868
6	1	0	-3.100563	3.107461	-2.836411
7	5	0	-1.841096	1.210843	-1.623959
8	1	0	-1.818060	0.589672	-2.624304
9	5	0	-2.309620	3.288980	0.993551
10	1	0	-2.586577	3.916614	1.956766
11	5	0	-1.532330	1.687326	1.190884
12	1	0	-1.292958	1.394364	2.311191
13	5	0	-0.703891	2.986862	0.326483
14	1	0	0.239740	3.537411	0.779409
15	5	0	-0.889313	2.691449	-1.416799
16	1	0	-0.063812	2.998853	-2.210501
17	5	0	-0.599444	1.297417	-0.310523
18	1	0	-3.552448	-1.181001	-2.060283
19	5	0	-3.078198	-1.528518	-1.033511
20	5	0	-4.021429	-2.773604	-0.160825
21	5	0	-2.403366	-3.137044	-0.769727
22	5	0	-1.338700	-1.695256	-0.588573
23	1	0	-5.062463	-3.125011	-0.598639
24	5	0	-3.905683	-2.464193	1.568469
25	5	0	-2.903424	-3.717088	0.840187
26	1	0	-2.238387	-3.888483	-1.672744
27	5	0	-1.276621	-3.034564	0.607625
28	5	0	-1.257090	-1.360958	1.184688
29	1	0	-4.817433	-2.521725	2.315945
30	5	0	-2.219219	-2.610569	2.042686
31	1	0	-3.101963	-4.858207	1.088206
32	1	0	-0.306579	-3.711103	0.687811
33	1	0	-0.364191	-0.923937	1.815638
34	1	0	-1.966099	-2.852839	3.171549
35	27	0	-2.305635	0.080299	0.080273
36	6	0	-3.878388	-1.190424	0.419157
37	6	0	-2.859836	-1.098612	1.661413
38	6	0	-3.313728	1.584601	-0.885242

39	6	0	-3.143179	1.853583	0.689890
40	1	0	-4.255447	1.180666	-1.226325
41	1	0	-3.986444	1.622975	1.326328
42	1	0	-4.781742	-0.598131	0.472834
43	1	0	-3.126284	-0.447040	2.480713
44	6	0	0.780582	0.572568	-0.427558
45	6	0	2.148971	1.202709	-0.138999
46	6	0	-0.079966	-1.549008	-1.564637
47	6	0	3.092513	0.110095	-0.490136
48	6	0	0.986874	-0.631664	-1.046169
49	6	0	2.424283	-0.936292	-1.098696
50	6	0	3.186193	-2.048394	-1.535278
51	6	0	4.414965	0.030717	-0.078707
52	1	0	-0.421048	-1.195767	-2.545579
53	1	0	0.352198	-2.540207	-1.737290
54	1	0	8.074109	-0.214037	1.101196
55	1	0	2.225141	1.976851	-0.928706
56	1	0	2.708863	-2.875916	-2.048503
57	6	0	4.546350	-2.089563	-1.277789
58	6	0	5.197006	-1.080549	-0.510461
59	6	0	4.890541	0.964786	0.893229
60	6	0	6.549933	-1.122947	-0.085136
61	1	0	5.131570	-2.938209	-1.618100
62	6	0	3.893525	1.847867	1.505025
63	6	0	6.209724	0.861344	1.295973
64	6	0	7.040524	-0.161524	0.776027
65	1	0	7.189769	-1.932944	-0.420583
66	1	0	6.603487	1.540732	2.045332
67	6	0	2.602566	1.904379	1.114768
68	1	0	4.217767	2.438736	2.357121
69	1	0	1.901527	2.541379	1.637759

Perylene

1	5	0	-4.837587	-2.607591	-0.000274
2	1	0	-5.998256	-2.821269	-0.000426
3	5	0	-3.446634	-3.685384	-0.000123
4	1	0	-3.604733	-4.859079	-0.000177
5	5	0	-3.809426	-2.695467	1.420590
6	1	0	-4.278805	-3.055958	2.443853
7	5	0	-2.692914	-1.296227	1.434605
8	1	0	-2.464795	-0.919861	2.524332
9	5	0	-3.809062	-2.695383	-1.420873
10	1	0	-4.278170	-3.055813	-2.444282
11	5	0	-2.692535	-1.296146	-1.434515
12	1	0	-2.464097	-0.919748	-2.524160
13	5	0	-2.132574	-2.878698	-0.888109
14	1	0	-1.376888	-3.503817	-1.550729
15	5	0	-2.132803	-2.878741	0.888259
16	1	0	-1.377319	-3.503918	1.551057
17	5	0	-1.588278	-1.400265	0.000175
18	1	0	-2.240160	1.192352	2.531079
19	5	0	-2.365882	1.616005	1.441916
20	5	0	-3.085983	3.251430	1.421528
21	5	0	-1.416834	2.999223	0.885907
22	5	0	-1.304097	1.434789	-0.000017
23	1	0	-3.454163	3.718438	2.443230
24	5	0	-4.103181	3.416628	0.000246
25	5	0	-2.483468	4.114383	0.000150
26	1	0	-0.503641	3.395469	1.529583
27	5	0	-1.416961	2.999272	-0.885838

28	5	0	-2.366095	1.616092	-1.441792
29	1	0	-5.174122	3.912744	0.000339
30	5	0	-3.086190	3.251514	-1.421193
31	1	0	-2.344645	5.290510	0.000173
32	1	0	-0.503867	3.395569	-1.529625
33	1	0	-2.240565	1.192527	-2.531012
34	1	0	-3.454522	3.718583	-2.442812
35	27	0	-3.003316	0.216420	0.000064
36	6	0	-3.905081	1.901527	0.800747
37	6	0	-3.905202	1.901574	-0.800370
38	6	0	-4.266147	-1.192251	0.800705
39	6	0	-4.265937	-1.192200	-0.801023
40	1	0	-5.072935	-0.677253	1.302447
41	1	0	-5.072590	-0.677167	-1.302944
42	1	0	-4.816898	1.605093	1.299655
43	1	0	-4.817101	1.605181	-1.299154
44	6	0	1.118938	-1.592129	0.000268
45	6	0	2.404180	-0.939715	0.000118
46	6	0	-0.094549	-0.824876	0.000185
47	6	0	3.605719	-1.716658	0.000196
48	6	0	2.464242	0.484095	-0.000107
49	6	0	0.010852	0.566033	-0.000014
50	6	0	4.915013	-1.038146	0.000038
51	6	0	3.509807	-3.101129	0.000423
52	6	0	3.765575	1.168160	-0.000278
53	6	0	1.270788	1.186394	-0.000150
54	6	0	4.966247	0.391392	-0.000200
55	6	0	1.101818	-3.009576	0.000501
56	6	0	3.874249	2.554747	-0.000517
57	1	0	1.284941	2.267799	-0.000294
58	1	0	8.382046	0.794963	-0.000410
59	1	0	8.266738	-1.680430	0.000006
60	6	0	6.114723	-1.741297	0.000105
61	6	0	7.357690	-1.088586	-0.000054
62	6	0	7.425461	0.283569	-0.000284
63	6	0	6.237495	1.054207	-0.000363
64	6	0	6.285913	2.469333	-0.000602
65	1	0	6.109463	-2.822228	0.000281
66	1	0	0.155664	-3.520718	0.000628
67	6	0	2.264940	-3.742116	0.000577
68	1	0	4.402177	-3.712406	0.000486
69	1	0	2.220905	-4.825763	0.000754
70	6	0	5.121094	3.198606	-0.000676
71	1	0	7.252651	2.961229	-0.000725
72	1	0	2.983114	3.166071	-0.000586
73	1	0	5.155669	4.282641	-0.000859

Perylene-extrusion

1	5	0	4.604455	-2.380128	-1.144377
2	1	0	5.757727	-2.548615	-1.330125
3	5	0	3.212873	-3.433265	-1.393323
4	1	0	3.361418	-4.528055	-1.819957
5	5	0	3.438487	-1.999878	-2.406110
6	1	0	3.804337	-1.971122	-3.529672
7	5	0	2.340475	-0.714284	-1.820096
8	1	0	1.999779	0.034510	-2.663605
9	5	0	3.722508	-2.999892	0.246423
10	1	0	4.298592	-3.683024	1.020899
11	5	0	2.631395	-1.719276	0.857897
12	1	0	2.516774	-1.691780	2.034447

13	5	0	2.003820	-3.027654	-0.152149
14	1	0	1.303856	-3.875035	0.285951
15	5	0	1.821819	-2.405625	-1.807283
16	1	0	0.973968	-2.784551	-2.544062
17	5	0	1.396813	-1.343190	-0.409379
18	1	0	3.299024	2.077785	-1.971289
19	5	0	2.933029	2.109578	-0.846751
20	5	0	3.658696	3.416909	0.135765
21	5	0	1.924355	3.397075	-0.190208
22	5	0	1.308923	1.701148	-0.173920
23	1	0	4.484791	4.112924	-0.345811
24	5	0	3.920850	2.816570	1.770418
25	5	0	2.522323	3.834519	1.429893
26	1	0	1.420799	4.203257	-0.900247
27	5	0	1.109637	2.765902	1.263824
28	5	0	1.615134	1.087249	1.497804
29	1	0	4.899944	3.010373	2.400542
30	5	0	2.356921	2.405670	2.463865
31	1	0	2.460878	4.931676	1.871828
32	1	0	0.026606	3.121752	1.587830
33	1	0	0.984838	0.322920	2.134306
34	1	0	2.246161	2.385314	3.640401
35	27	0	2.791371	0.197989	0.009981
36	6	0	4.026633	1.786709	0.403057
37	6	0	3.289397	1.215560	1.715676
38	6	0	3.962924	-0.794731	-1.347433
39	6	0	4.126249	-1.361530	0.149957
40	1	0	4.709831	-0.101460	-1.705102
41	1	0	4.981519	-1.022723	0.718634
42	1	0	5.046078	1.469871	0.230105
43	1	0	3.847688	0.543777	2.351129
44	6	0	-0.115872	-1.012856	-0.205373
45	6	0	-1.176738	-2.017385	0.213131
46	6	0	-0.026722	1.395949	-1.002187
47	6	0	-2.445316	-1.241439	0.120514
48	6	0	-0.747874	0.142144	-0.587123
49	6	0	-2.207970	-0.012688	-0.431005
50	6	0	-3.347691	0.844933	-0.733703
51	6	0	-3.663964	-1.651352	0.725208
52	1	0	0.203150	1.361862	-2.074688
53	1	0	-0.685104	2.253355	-0.860161
54	1	0	-2.294622	-3.914564	2.870874
55	1	0	-1.166464	-2.734692	-0.635787
56	6	0	-3.258732	2.017609	-1.472496
57	6	0	-4.651656	0.407365	-0.288119
58	6	0	-4.839977	-0.822125	0.430250
59	6	0	-3.589498	-2.662668	1.656123
60	6	0	-6.122588	-1.194996	0.812448
61	6	0	-5.795481	1.214616	-0.580887
62	6	0	-2.311761	-3.221783	2.035163
63	1	0	-4.466174	-2.967424	2.215177
64	1	0	-6.269801	-2.136773	1.326852
65	6	0	-7.235050	-0.388136	0.534121
66	1	0	-0.202878	-3.292058	1.770919
67	6	0	-1.145499	-2.880189	1.437495
68	1	0	-2.301001	2.330766	-1.857436
69	6	0	-4.392382	2.804062	-1.751044
70	6	0	-5.634023	2.423679	-1.309485
71	6	0	-7.077085	0.796900	-0.147945
72	1	0	-8.221537	-0.708417	0.851299

73	1	0	-7.933105	1.424064	-0.373425
74	1	0	-6.509750	3.029633	-1.515816
75	1	0	-4.272874	3.717704	-2.323031

Figure S6. Comparison of aromaticity of linear benzenoids linked and non-linked to [*o*-COSAN]$^-$. [*o*-COSAN]$^-$ without (left) and with extrusion (right). NICS (in ppm) and MCI values (in italics and in au) for the benzenoid moiety are included in the center of the rings, whereas those for the fully relaxed benzenoids not linked to [*o*-COSAN]$^-$ are depicted outside the rings.

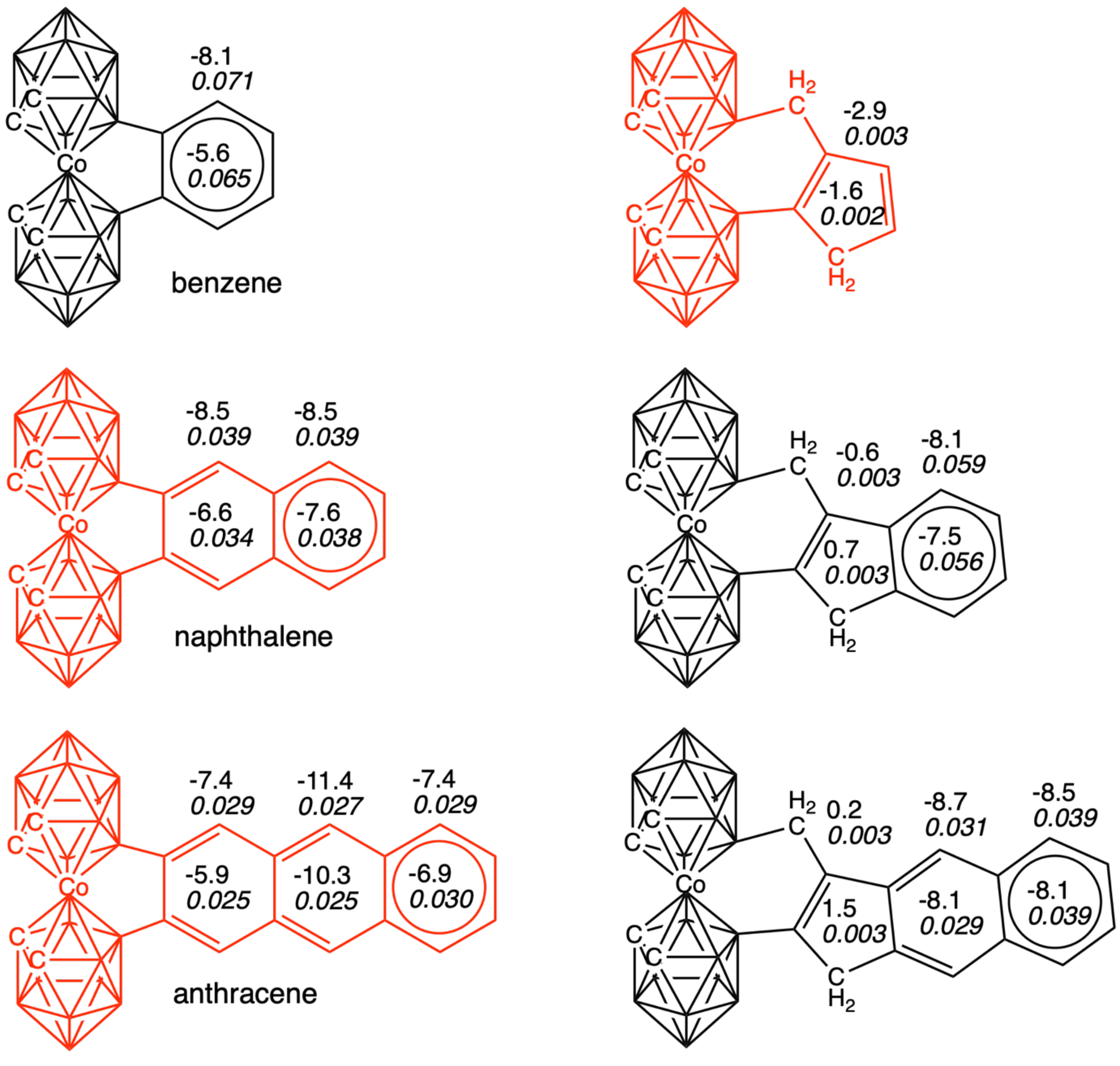


Figure S7. Comparison of aromaticity of kinked benzenoids linked and non-linked to [*o*-COSAN]$^-$. [*o*-COSAN]$^-$ without (left) and with extrusion (right). NICS (in ppm) and MCI values (in italics and in au) for the benzenoid moiety are included in the center of the rings, whereas those for the fully relaxed benzenoids not linked to [*o*-COSAN]$^-$ are depicted outside the rings.

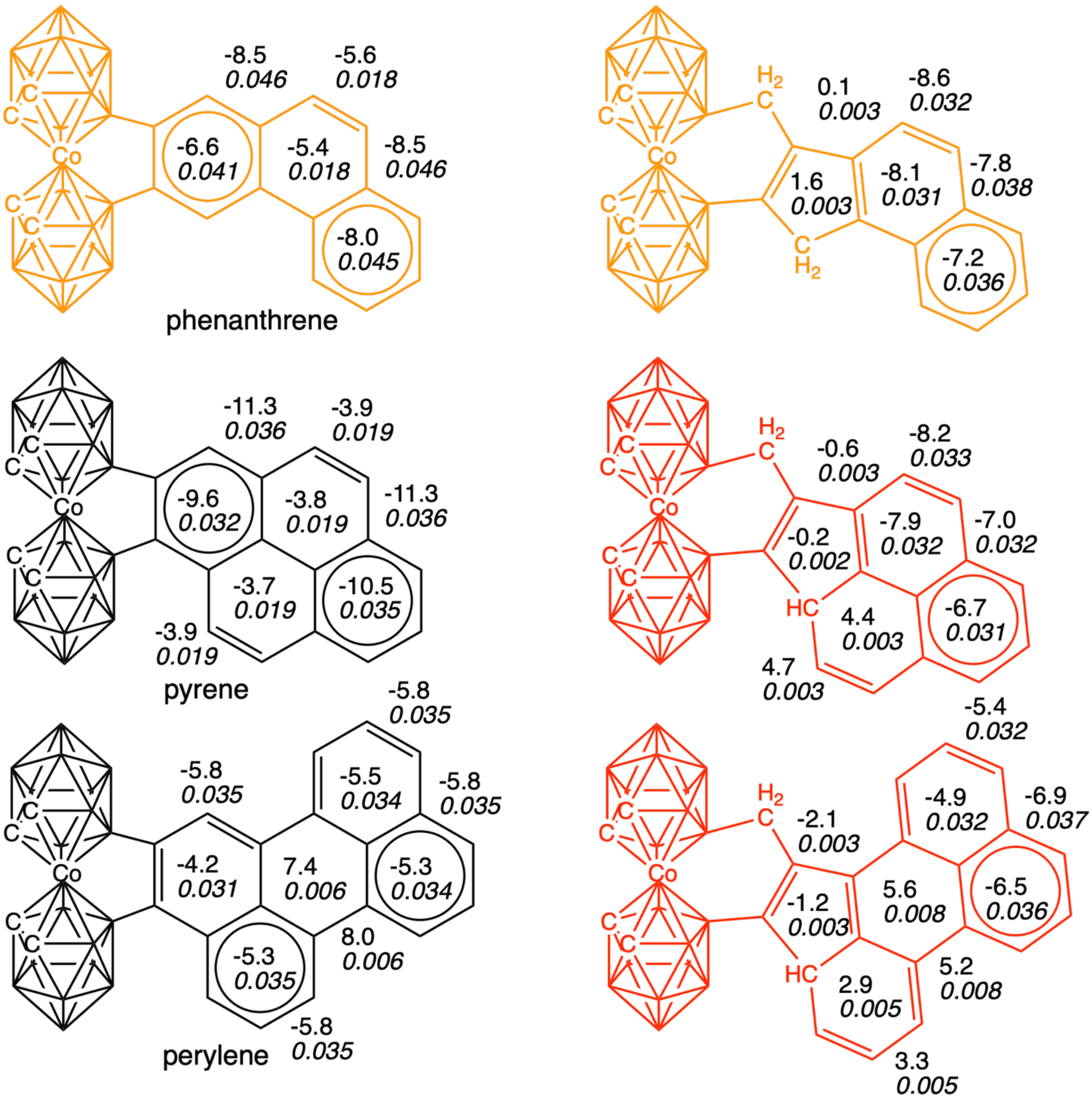
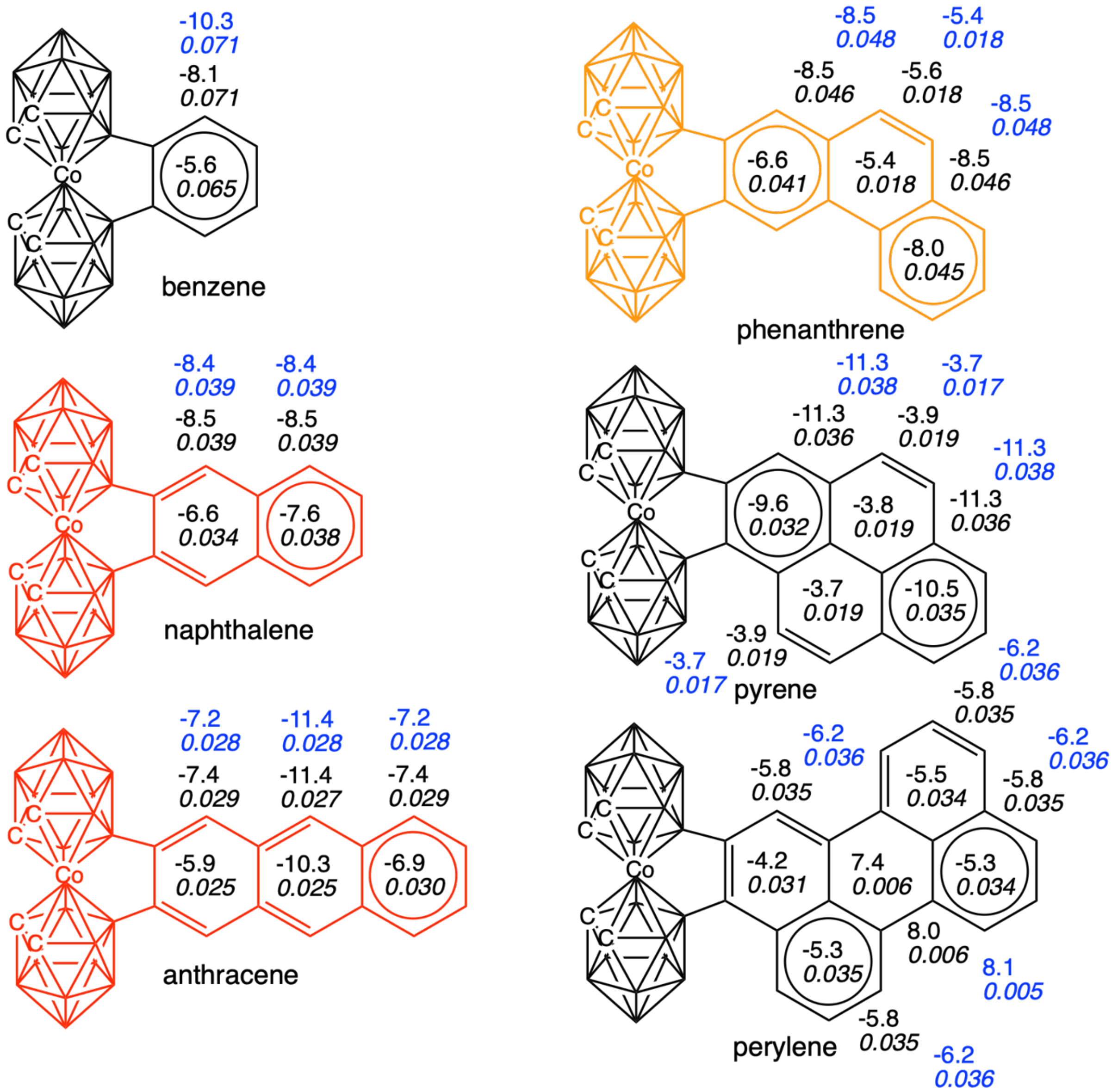


Table S3: Extrusion energies (in kcal mol^{-1}) computed based on two different reactions: (1) [o-COSAN]$^-$-benzenoid + H_2 → [o-COSAN]$^-$-benzenoid^{extruded}; and (2) [o-COSAN]$^-$ + benzenoid → [o-COSAN]$^-$-benzenoid^{extruded} + H_2. Distances (in Å) between the two B atoms fused to the benzenoid are also included.[a,b]

	ΔE_{ext}^1	ΔG_{ext}^1	ΔE_{ext}^2	ΔG_{ext}^2
benzene	3.1	16.3	12.2	14.8
naphthalene	-7.1	6.2	-0.5	1.9
anthracene	-11.1	4.1	-6.0	-1.6
phenanthrene	-5.6	7.5	0.0	3.7
pyrene	17.3	31.4	24.9	29.3
perylene	22.5	36.7	29.5	33.7

[a] The equivalent distance between the two B atoms in [*o*-COSAN]$^-$ is 3.144 Å. [b] Extrusion energies calculated at the BLYP-D3BJ/TZ2P//B3LYP(GD3BJ)/6-311++G** level of theory by means of AMS software.

Figure S8. Comparison of aromaticity of linear and kinked benzenoids linked and non-linked to [*o*-COSAN]$^-$ without extrusion. NICS (in ppm) and MCI values (in italics and in au) for the benzenoid moiety are included in the center of the rings, whereas those for the fully relaxed benzenoids not linked to [*o*-COSAN]$^-$ are depicted outside the rings, at the same B3LYP/6-311++G** level of theory (in black) and at the CAM-B3LYP/6-311++G** (in blue).



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