Supplementary Material (ESI) for PCCP

–Supporting Information–

Charge-transport properties of prototype molecular materials for organic electronics based on graphene nanoribbons

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Absolute energies and XYZ coordinates of the stationary states found[1]

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[1]Note that we have chosen a cofacially stacked dimeric nanostructure to approximate the expected thin-films packing; the pair of molecules in its ground state are separated exactly by 3.5 Å and can be thus built directly from the XYZ coordinates of the monomers presented here.

Table S1: XYZ coordinates (in Å) for the fully optimized structure of circumbenzene at the B3LYP level[a]

C	1.011219	1.011219	0.000000
C	1.379873	−0.369683	0.000000
C	0.369683	−1.379873	0.000000
C	−1.011219	−1.011219	0.000000
C	−1.379873	0.369683	0.000000
C	−0.369683	1.379873	0.000000
C	2.017209	2.017209	0.000000
C	3.386435	1.618846	0.000000
C	3.740802	0.291334	0.000000
C	2.754644	−0.737282	0.000000
C	3.093564	−2.121695	0.000000
C	2.121695	−3.093564	0.000000
C	0.737282	−2.754644	0.000000
C	−0.291334	−3.740802	0.000000
C	−1.618846	−3.386435	0.000000
C	−2.017209	−2.017209	0.000000
C	−3.386435	−1.618846	0.000000
C	−3.740802	−0.291334	0.000000
C	−2.754644	0.737282	0.000000
C	−3.093564	2.121695	0.000000
C	−2.121695	3.093564	0.000000
C	−0.737282	2.754644	0.000000
C	0.291334	3.740802	0.000000
C	1.618846	3.386435	0.000000
H	2.393191	4.157464	0.000000
H	4.157464	2.393191	0.000000
H	4.795418	0.004989	0.000000
H	4.149652	−2.402529	0.000000
H	2.402529	−4.149652	0.000000
H	−0.004989	−4.795418	0.000000
H	−2.393191	−4.157464	0.000000
H	−4.157464	−2.393191	0.000000
H	−4.795418	−0.004989	0.000000
H	−4.149652	2.402529	0.000000
H	−2.402529	4.149652	0.000000
H	0.004989	4.795418	0.000000

[a] Final energy (in a.u.): -921.401712049.

Table S2: XYZ coordinates (in Å) for the fully optimized structure of circumnaphtalene at the B3LYP level[a]

C	−0.718214	0.000000	0.000000
C	−1.426973	1.229901	0.000000
C	−0.714205	2.467916	0.000000
C	−1.424984	3.701744	0.000000
C	−0.691050	4.913119	0.000000
C	−2.859677	3.670042	0.000000
C	−3.545191	2.487754	0.000000
C	−2.860400	1.226009	0.000000
C	−3.540880	0.000000	0.000000
C	−2.860400	−1.226009	0.000000
C	−3.545191	−2.487754	0.000000
C	−2.859677	−3.670042	0.000000
C	−1.424984	−3.701744	0.000000
C	−1.426973	−1.229901	0.000000
C	−0.691050	−4.913119	0.000000
C	−0.714205	−2.467916	0.000000
C	0.691050	−4.913119	0.000000
C	0.714205	−2.467916	0.000000
C	0.718214	0.000000	0.000000
C	0.714205	2.467916	0.000000
C	0.691050	4.913119	0.000000
C	1.424984	−3.701744	0.000000
C	1.426973	−1.229901	0.000000
C	1.426973	1.229901	0.000000
C	1.424984	3.701744	0.000000
C	2.859677	−3.670042	0.000000
C	2.860400	−1.226009	0.000000
C	2.860400	1.226009	0.000000
C	2.859677	3.670042	0.000000
C	3.545191	−2.487754	0.000000
C	3.540880	0.000000	0.000000
C	3.545191	2.487754	0.000000
H	−4.634271	0.000000	0.000000
H	−4.637912	2.485060	0.000000
H	−4.637912	−2.485060	0.000000
H	−3.400858	4.619411	0.000000
H	−3.400858	−4.619411	0.000000
H	−1.237317	5.859539	0.000000
H	−1.237317	−5.859539	0.000000
H	1.237317	−5.859539	0.000000
H	3.400858	−4.619411	0.000000
H	4.637912	−2.485060	0.000000
H	4.634271	0.000000	0.000000
H	4.637912	2.485060	0.000000
H	3.400858	4.619411	0.000000
H	1.237317	5.859539	0.000000

[a] Final energy (in a.u.): -1227.353054366.

Table S3: XYZ coordinates (in Å) for the fully optimized structure of circumanthracene at the B3LYP level[a]

C	3.546097	2.487707	0.000000
C	2.861824	1.220979	0.000000
C	1.421674	1.226825	0.000000
C	0.710922	2.462936	0.000000
C	1.422412	3.699275	0.000000
C	2.860780	3.666812	0.000000
C	0.712807	−0.000433	0.000000
C	−0.723979	0.000746	0.000000
C	−1.430819	1.229137	0.000000
C	−0.718010	2.464086	0.000000
C	−2.870983	1.225683	0.000000
C	−3.551823	0.010143	0.000000
C	−2.871932	−1.229934	0.000000
C	−1.433507	−1.231128	0.000000
C	1.420299	−1.233461	0.000000
C	0.710768	−2.465338	0.000000
C	−0.726020	−2.464155	0.000000
C	−3.553198	2.493525	0.000000
C	−2.865879	3.671459	0.000000
C	−1.427469	3.701542	0.000000
C	0.692108	4.906273	0.000000
C	−0.695176	4.907323	0.000000
C	−1.434873	−3.691417	0.000000
C	−2.875026	−3.685593	0.000000
C	−3.553799	−2.468967	0.000000
C	1.417597	−3.693729	0.000000
C	0.704808	−4.928690	0.000000
C	−0.724129	−4.927533	0.000000
C	2.858723	−1.234668	0.000000
C	3.538611	−2.474755	0.000000
C	2.857759	−3.690284	0.000000
C	3.540603	0.004354	0.000000
H	−4.645039	0.010949	0.000000
H	−4.645866	2.492750	0.000000
H	−4.647020	−2.467909	0.000000
H	−3.404097	4.622513	0.000000
H	−1.239085	5.855066	0.000000
C	−1.435645	−6.163857	0.000000
C	1.414258	−6.166141	0.000000
H	4.631827	−2.475522	0.000000
H	4.633822	0.003353	0.000000
H	4.638765	2.485112	0.000000
H	3.400610	4.616950	0.000000
H	1.237514	5.853150	0.000000
C	2.852681	−6.136063	0.000000
C	0.681961	−7.371907	0.000000
H	3.390876	−7.087129	0.000000
C	3.539987	−4.958125	0.000000
H	4.632656	−4.957337	0.000000
C	−0.705336	−7.370844	0.000000
C	−2.874017	−6.131410	0.000000
H	−1.250643	−8.317779	0.000000
H	1.225774	−8.319705	0.000000
C	−3.559331	−4.952307	0.000000
H	−3.413775	−7.081588	0.000000
H	−4.651998	−4.949650	0.000000

[a] Final energy (in a.u.): -1533.298606004.

Table S4: XYZ coordinates (in Å) for the fully optimized structure of circumtetracene at the B3LYP level[a]

C	−3.569345	−4.921196	0.000000
C	−2.884837	−3.676558	0.000000
C	−1.441918	−3.681102	0.000000
C	−0.736234	−4.915424	0.000000
C	−1.447890	−6.142496	0.000000
C	−3.563202	−2.445206	0.000000
C	−2.878016	−1.217612	0.000000
C	−1.435123	−1.221035	0.000000
C	−0.730002	−2.453019	0.000000
C	−0.722605	0.009330	0.000000
C	−1.427381	1.240314	0.000000
C	−2.870413	1.240033	0.000000
C	−3.555494	0.030808	0.000000
C	−0.712280	2.471168	0.000000
C	0.717541	2.467206	0.000000
C	1.425800	1.232403	0.000000
C	0.714196	0.005348	0.000000
C	1.431182	3.704981	0.000000
C	2.870465	3.670617	0.000000
C	3.555100	2.492517	0.000000
C	2.868806	1.224125	0.000000
C	1.419878	−1.228943	0.000000
C	2.862806	−1.233524	0.000000
C	3.547190	0.011121	0.000000
C	−1.419047	3.712879	0.000000
C	−0.685740	4.914516	0.000000
C	0.704549	4.910664	0.000000
C	0.707927	−2.456992	0.000000
C	−3.549662	2.512211	0.000000
C	−2.858499	3.686492	0.000000
C	3.541172	−2.464909	0.000000
C	2.855950	−3.692457	0.000000
C	1.413033	−3.688971	0.000000
C	0.700570	−4.919369	0.000000
C	3.533388	−4.940920	0.000000
C	2.848364	−6.150150	0.000000
C	1.405309	−6.150329	0.000000
C	0.690190	−7.381246	0.000000
H	−4.648575	0.034816	0.000000
H	−4.642280	2.514506	0.000000
H	−4.656167	−2.441933	0.000000
H	−3.393101	4.639639	0.000000
H	−1.226818	5.863871	0.000000
H	4.634138	−2.467739	0.000000
H	4.640276	0.009077	0.000000
H	4.647715	2.488745	0.000000
H	3.410344	4.620784	0.000000
H	1.250883	5.857004	0.000000
H	4.626471	−4.944548	0.000000
C	1.397111	−8.622931	0.000000
H	−4.662413	−4.918820	0.000000
C	0.663837	−9.824511	0.000000
C	2.836525	−8.596558	0.000000
H	1.204595	−10.774038	0.000000
C	−0.726560	−9.820616	0.000000
H	−1.272686	−10.767085	0.000000
C	−1.453270	−8.615072	0.000000
C	3.527719	−7.422299	0.000000
H	3.371184	−9.549671	0.000000
H	4.620327	−7.424794	0.000000
C	−0.739542	−7.377205	0.000000
C	−2.892464	−8.580544	0.000000
H	−3.432607	−9.530579	0.000000
C	−3.577263	−7.402467	0.000000
C	−2.890887	−6.134085	0.000000
H	−4.669859	−7.399181	0.000000

[a] Final energy (in a.u.): -1839.241237072.

Table S5: XYZ coordinates (in Å) for the fully optimized structure of circumbenzene at the B2-PLYP level[a]

C	1.010840	1.010840	0.000000
C	1.379919	−0.369723	0.000000
C	0.369723	−1.379919	0.000000
C	−1.010840	−1.010839	0.000000
C	−1.379919	0.369723	0.000000
C	−0.369723	1.379919	0.000000
C	2.017282	2.017282	0.000000
C	3.386766	1.620102	0.000000
C	3.742264	0.290354	0.000000
C	2.755107	−0.737778	0.000000
C	3.095395	−2.122094	0.000000
C	2.122094	−3.095395	0.000000
C	0.737778	−2.755107	0.000000
C	−0.290354	−3.742264	0.000000
C	−1.620102	−3.386766	0.000000
C	−2.017282	−2.017282	0.000000
C	−3.386766	−1.620102	0.000000
C	−3.742264	−0.290354	0.000000
C	−2.755107	0.737778	0.000000
C	−3.095395	2.122094	0.000000
C	−2.122094	3.095395	0.000000
C	−0.737778	2.755107	0.000000
C	0.290354	3.742264	0.000000
C	1.620102	3.386766	0.000000
H	2.394298	4.156989	0.000000
H	4.156989	2.394297	0.000000
H	4.796221	0.004227	0.000000
H	4.150932	−2.402328	0.000000
H	2.402328	−4.150932	0.000000
H	−0.004227	−4.796221	0.000000
H	−2.394297	−4.156989	0.000000
H	−4.156989	−2.394298	0.000000
H	−4.796221	−0.004227	0.000000
H	−4.150932	2.402328	0.000000
H	−2.402328	4.150932	0.000000
H	0.004227	4.796221	0.000000

[a] Final energy (in a.u.): -921.255756454.

Table S6: XYZ coordinates (in Å) for the fully optimized structure of circumnaphtalene at the B2-PLYP level[a]

C	−0.717442	0.000000	0.000000
C	−1.427400	1.230429	0.000000
C	−0.714411	2.467567	0.000000
C	−1.425395	3.701954	0.000000
C	−0.691979	4.914384	0.000000
C	−2.859431	3.671833	0.000000
C	−3.546989	2.487194	0.000000
C	−2.860964	1.226493	0.000000
C	−3.543723	0.000000	0.000000
C	−2.860964	−1.226493	0.000000
C	−3.546989	−2.487194	0.000000
C	−2.859431	−3.671833	0.000000
C	−1.425395	−3.701954	0.000000
C	−1.427400	−1.230429	0.000000
C	−0.691979	−4.914384	0.000000
C	−0.714411	−2.467566	0.000000
C	0.691979	−4.914384	0.000000
C	0.714412	−2.467566	0.000000
C	0.717442	0.000000	0.000000
C	0.714412	2.467567	0.000000
C	0.691978	4.914384	0.000000
C	1.425395	−3.701954	0.000000
C	1.427400	−1.230429	0.000000
C	1.427400	1.230429	0.000000
C	1.425395	3.701954	0.000000
C	2.859431	−3.671833	0.000000
C	2.860965	−1.226493	0.000000
C	2.860965	1.226493	0.000000
C	2.859431	3.671833	0.000000
C	3.546989	−2.487194	0.000000
C	3.543723	0.000000	0.000000
C	3.546989	2.487194	0.000000
H	−4.636772	0.000000	0.000000
H	−4.639051	2.484908	0.000000
H	−4.639050	−2.484909	0.000000
H	−3.400245	4.620640	0.000000
H	−3.400244	−4.620640	0.000000
H	−1.238392	5.859974	0.000000
H	−1.238392	−5.859974	0.000000
H	1.238391	−5.859974	0.000000
H	3.400244	−4.620640	0.000000
H	4.639050	−2.484909	0.000000
H	4.636773	0.000000	0.000000
H	4.639051	2.484909	0.000000
H	3.400244	4.620640	0.000000
H	1.238391	5.859974	0.000000

[a] Final energy (in a.u.): -1227.166766562.

Table S7: XYZ coordinates (in Å) for the fully optimized structure of circumanthracene at the B2-PLYP level[a]

C	3.547422	2.486976	0.000000
C	2.861723	1.222110	0.000000
C	1.422426	1.228008	0.000000
C	0.711363	2.463012	0.000000
C	1.422962	3.699786	0.000000
C	2.860128	3.669047	0.000000
C	0.711968	−0.000810	0.000000
C	−0.723146	0.000370	0.000000
C	−1.431581	1.230339	0.000000
C	−0.718471	2.464176	0.000000
C	−2.870888	1.226825	0.000000
C	−3.554445	0.009842	0.000000
C	−2.872907	−1.229932	0.000000
C	−1.433650	−1.231128	0.000000
C	1.420438	−1.233468	0.000000
C	0.709934	−2.464966	0.000000
C	−0.725180	−2.463786	0.000000
C	−3.554521	2.492811	0.000000
C	−2.865244	3.673725	0.000000
C	−1.428036	3.702092	0.000000
C	0.692822	4.908316	0.000000
C	−0.695905	4.909413	0.000000
C	−1.435636	−3.692604	0.000000
C	−2.874934	−3.686709	0.000000
C	−3.556455	−2.468625	0.000000
C	1.418367	−3.694935	0.000000
C	0.705260	−4.928774	0.000000
C	−0.724574	−4.927609	0.000000
C	2.859695	−1.234666	0.000000
C	3.541233	−2.474442	0.000000
C	2.857675	−3.691423	0.000000
C	3.543245	0.004024	0.000000
H	−4.647450	0.011091	0.000000
H	−4.646557	2.492019	0.000000
H	−4.649463	−2.468057	0.000000
H	−3.403162	4.624175	0.000000
H	−1.240070	5.856293	0.000000
C	−1.436179	−6.164380	0.000000
C	1.414826	−6.166690	0.000000
H	4.634238	−2.475679	0.000000
H	4.636253	0.003471	0.000000
H	4.639456	2.484377	0.000000
H	3.399639	4.618592	0.000000
H	1.238515	5.854313	0.000000
C	2.852036	−6.138324	0.000000
C	0.682691	−7.374006	0.000000
H	3.389945	−7.088778	0.000000
C	3.541310	−4.957409	0.000000
H	4.633345	−4.956613	0.000000
C	−0.706039	−7.372906	0.000000
C	−2.873347	−6.133643	0.000000
H	−1.251704	−8.318920	0.000000
H	1.226829	−8.320902	0.000000
C	−3.560638	−4.951574	0.000000
H	−3.412838	−7.083200	0.000000
H	−4.652672	−4.948956	0.000000

[a] Final energy (in a.u.): -1533.071999865.

Table S8: XYZ coordinates (in Å) for the fully optimized structure of circumtetracene at the B2-PLYP level[a]

C	−3.570324	−4.920105	0.000000
C	−2.884902	−3.677452	0.000000
C	−1.441679	−3.682150	0.000000
C	−0.735541	−4.915009	0.000000
C	−1.448748	−6.144469	0.000000
C	−3.564880	−2.445164	0.000000
C	−2.878082	−1.216660	0.000000
C	−1.434854	−1.219963	0.000000
C	−0.728474	−2.453025	0.000000
C	−0.721888	0.008958	0.000000
C	−1.428266	1.242353	0.000000
C	−2.869290	1.242005	0.000000
C	−3.556600	0.029774	0.000000
C	−0.712915	2.472190	0.000000
C	0.718176	2.468222	0.000000
C	1.426696	1.234437	0.000000
C	0.713490	0.004978	0.000000
C	1.431831	3.705898	0.000000
C	2.869393	3.673291	0.000000
C	3.555508	2.491371	0.000000
C	2.867696	1.226099	0.000000
C	1.419631	−1.227878	0.000000
C	2.862854	−1.232578	0.000000
C	3.548272	0.010074	0.000000
C	−1.419693	3.713806	0.000000
C	−0.685979	4.917687	0.000000
C	0.704804	4.913830	0.000000
C	0.706423	−2.457003	0.000000
C	−3.550073	2.511073	0.000000
C	−2.857415	3.689170	0.000000
C	3.542830	−2.464872	0.000000
C	2.856030	−3.693369	0.000000
C	1.412802	−3.690063	0.000000
C	0.699839	−4.918989	0.000000
C	3.534550	−4.939806	0.000000
C	2.847243	−6.152036	0.000000
C	1.406217	−6.152384	0.000000
C	0.690865	−7.382221	0.000000
H	−4.649559	0.034026	0.000000
H	−4.642101	2.513023	0.000000
H	−4.657804	−2.442112	0.000000
H	−3.392243	4.641418	0.000000
H	−1.227520	5.866104	0.000000
H	4.635755	−2.467879	0.000000
H	4.641239	0.008266	0.000000
H	4.647529	2.487264	0.000000
H	3.409492	4.622558	0.000000
H	1.251599	5.859229	0.000000
H	4.627509	−4.944019	0.000000
C	1.397648	−8.623837	0.000000
H	−4.663290	−4.918264	0.000000
C	0.663936	−9.827714	0.000000
C	2.835369	−8.599199	0.000000
H	1.205439	−10.776153	0.000000
C	−0.726851	−9.823859	0.000000
H	−1.273615	−10.769275	0.000000
C	−1.453881	−8.615935	0.000000
C	3.528028	−7.421101	0.000000
H	3.370201	−9.551444	0.000000
H	4.620056	−7.423065	0.000000
C	−0.740226	−7.378254	0.000000
C	−2.891440	−8.583320	0.000000
H	−3.431572	−9.532569	0.000000
C	−3.577556	−7.401399	0.000000
C	−2.889750	−6.136128	0.000000
H	−4.669578	−7.397342	0.000000

[a] Final energy (in a.u.): -1838.974802720.

Table S9: XYZ coordinates (in Å) for the fully optimized structure of circumbenzene at the B3LYP level[a]

C	1.419983	0.000000	0.000000
C	−1.419983	0.000000	0.000000
C	0.709230	−1.234190	0.000000
C	−0.709231	1.234190	0.000000
C	0.709230	1.234190	0.000000
C	−0.709231	−1.234190	0.000000
C	1.426349	−2.476561	0.000000
C	−1.426349	2.476562	0.000000
C	1.426349	2.476561	0.000000
C	−1.426349	−2.476561	0.000000
C	0.682732	−3.708147	0.000000
C	−0.682732	3.708147	0.000000
C	0.682732	3.708147	0.000000
C	−0.682732	−3.708147	0.000000
C	2.841272	0.000000	0.000000
C	−2.841272	0.000000	0.000000
C	3.526746	−1.244725	0.000000
C	−3.526746	1.244725	0.000000
C	3.526746	1.244725	0.000000
C	−3.526746	−1.244725	0.000000
C	2.836834	−2.449994	0.000000
C	−2.836834	2.449994	0.000000
C	2.836834	2.449994	0.000000
C	−2.836834	−2.449994	0.000000
H	4.618980	−1.246786	0.000000
H	−4.618980	1.246786	0.000000
H	4.618980	1.246786	0.000000
H	−4.618980	−1.246786	0.000000
H	3.388834	−3.391608	0.000000
H	−3.388834	3.391608	0.000000
H	3.388834	3.391608	0.000000
H	−3.388834	−3.391608	0.000000
H	1.234658	−4.649922	0.000000
H	−1.234658	4.649922	0.000000
H	1.234658	4.649922	0.000000
H	−1.234658	−4.649922	0.000000

[a] Final energy (in a.u.): -921.148932110.

Table S10: XYZ coordinates (in Å) for the fully optimized structure of circumnaphtalene at the B3LYP level[a]

C	−0.711989	0.000000	0.000000
C	−1.422499	1.234343	0.000000
C	−0.712895	2.465628	0.000000
C	−1.426654	3.701051	0.000000
C	−0.686506	4.924003	0.000000
C	−2.849649	3.675431	0.000000
C	−3.539714	2.483517	0.000000
C	−2.852035	1.232543	0.000000
C	−3.534944	0.000000	0.000000
C	−2.852035	−1.232543	0.000000
C	−3.539714	−2.483517	0.000000
C	−2.849649	−3.675431	0.000000
C	−1.426654	−3.701051	0.000000
C	−1.422499	−1.234343	0.000000
C	−0.686506	−4.924003	0.000000
C	−0.712895	−2.465628	0.000000
C	0.686506	−4.924002	0.000000
C	0.712895	−2.465628	0.000000
C	0.711988	0.000000	0.000000
C	0.712895	2.465628	0.000000
C	0.686506	4.924003	0.000000
C	1.426654	−3.701051	0.000000
C	1.422499	−1.234343	0.000000
C	1.422499	1.234343	0.000000
C	1.426654	3.701051	0.000000
C	2.849649	−3.675431	0.000000
C	2.852035	−1.232543	0.000000
C	2.852035	1.232543	0.000000
C	2.849649	3.675431	0.000000
C	3.539714	−2.483517	0.000000
C	3.534944	0.000000	0.000000
C	3.539714	2.483517	0.000000
H	−4.627927	0.000000	0.000000
H	−4.631661	2.484320	0.000000
H	−4.631661	−2.484320	0.000000
H	−3.394368	4.621539	0.000000
H	−3.394368	−4.621539	0.000000
H	−1.234401	5.868358	0.000000
H	−1.234401	−5.868357	0.000000
H	1.234401	−5.868358	0.000000
H	3.394368	−4.621539	0.000000
H	4.631661	−2.484320	0.000000
H	4.627927	0.000000	0.000000
H	4.631661	2.484320	0.000000
H	3.394368	4.621539	0.000000
H	1.234401	5.868358	0.000000

[a] Final energy (in a.u.): -1227.124464781.

Table S11: XYZ coordinates (in Å) for the fully optimized structure of circumanthracene at the B3LYP level[a]

C	3.543165	2.483818	0.000000
C	2.855120	1.227502	0.000000
C	1.420651	1.229305	0.000000
C	0.710745	2.461441	0.000000
C	1.423955	3.694776	0.000000
C	2.854034	3.668832	0.000000
C	0.709201	−0.003441	0.000000
C	−0.720389	−0.002260	0.000000
C	−1.429812	1.231629	0.000000
C	−0.717838	2.462599	0.000000
C	−2.864289	1.232222	0.000000
C	−3.548225	0.006942	0.000000
C	−2.865541	−1.229941	0.000000
C	−1.428095	−1.231135	0.000000
C	1.414884	−1.233459	0.000000
C	0.707177	−2.462333	0.000000
C	−0.722415	−2.461152	0.000000
C	−3.550285	2.489646	0.000000
C	−2.859116	3.673483	0.000000
C	−1.429009	3.697061	0.000000
C	0.687719	4.911650	0.000000
C	−0.690766	4.912716	0.000000
C	−1.433859	−3.693900	0.000000
C	−2.868326	−3.692105	0.000000
C	−3.550236	−2.465771	0.000000
C	1.416596	−3.696223	0.000000
C	0.704629	−4.927199	0.000000
C	−0.723954	−4.926037	0.000000
C	2.852329	−1.234661	0.000000
C	3.535013	−2.471544	0.000000
C	2.851071	−3.696821	0.000000
C	3.537026	0.001168	0.000000
H	−4.641027	0.008302	0.000000
H	−4.642143	2.490952	0.000000
H	−4.643040	−2.465322	0.000000
H	−3.398654	4.622693	0.000000
H	−1.235540	5.859019	0.000000
C	−1.437176	−6.159364	0.000000
C	1.415801	−6.161656	0.000000
H	4.627815	−2.472899	0.000000
H	4.629830	0.000730	0.000000
H	4.635027	2.483289	0.000000
H	3.395183	4.617123	0.000000
H	1.234006	5.857076	0.000000
C	2.845913	−6.138082	0.000000
C	0.677552	−7.377305	0.000000
H	3.385425	−7.087307	0.000000
C	3.537073	−4.954244	0.000000
H	4.628931	−4.955538	0.000000
C	−0.700937	−7.376235	0.000000
C	−2.867259	−6.133430	0.000000
H	−1.247185	−8.321684	0.000000
H	1.222288	−8.323629	0.000000
C	−3.556384	−4.948416	0.000000
H	−3.408364	−7.081745	0.000000
H	−4.648246	−4.947850	0.000000

[a] Final energy (in a.u.): -1533.086770949.

Table S12: XYZ coordinates (in Å) for the fully optimized structure of circumtetracene at the B3LYP level[a]

C	−3.567392	−4.916371	0.000000
C	−2.879138	−3.679752	0.000000
C	−1.438113	−3.682405	0.000000
C	−0.734732	−4.911630	0.000000
C	−1.448691	−6.141807	0.000000
C	−3.560342	−2.445217	0.000000
C	−2.872332	−1.214494	0.000000
C	−1.431318	−1.219767	0.000000
C	−0.726707	−2.453029	0.000000
C	−0.721149	0.005525	0.000000
C	−1.428220	1.239629	0.000000
C	−2.865907	1.244480	0.000000
C	−3.553630	0.025958	0.000000
C	−0.712124	2.469417	0.000000
C	0.717356	2.465455	0.000000
C	1.426619	1.231713	0.000000
C	0.712707	0.001548	0.000000
C	1.432191	3.698143	0.000000
C	2.865984	3.669997	0.000000
C	3.554059	2.488705	0.000000
C	2.864307	1.228597	0.000000
C	1.416075	−1.227656	0.000000
C	2.857122	−1.230374	0.000000
C	3.545278	0.006284	0.000000
C	−1.420114	3.706047	0.000000
C	−0.681797	4.915694	0.000000
C	0.700591	4.911864	0.000000
C	0.704620	−2.456988	0.000000
C	−3.548660	2.508392	0.000000
C	−2.854039	3.685847	0.000000
C	3.538325	−2.464890	0.000000
C	2.850261	−3.695607	0.000000
C	1.409233	−3.690243	0.000000
C	0.699120	−4.915568	0.000000
C	3.531536	−4.936071	0.000000
C	2.843835	−6.154624	0.000000
C	1.406167	−6.149655	0.000000
C	0.690016	−7.379484	0.000000
H	−4.646220	0.029671	0.000000
H	−4.640474	2.512178	0.000000
H	−4.653072	−2.442074	0.000000
H	−3.388458	4.638100	0.000000
H	−1.223138	5.864069	0.000000
H	4.631063	−2.467808	0.000000
H	4.637878	0.003952	0.000000
H	4.645880	2.486428	0.000000
H	3.405672	4.619273	0.000000
H	1.247181	5.857224	0.000000
H	4.624133	−4.939553	0.000000
C	1.398133	−8.616071	0.000000
H	−4.659972	−4.913869	0.000000
C	0.659826	−9.825667	0.000000
C	2.832049	−8.595933	0.000000
H	1.200968	−10.774153	0.000000
C	−0.722609	−9.821785	0.000000
H	−1.269127	−10.767194	0.000000
C	−1.454266	−8.608123	0.000000
C	3.526700	−7.418485	0.000000
H	3.366484	−9.548175	0.000000
H	4.618509	−7.422355	0.000000
C	−0.739388	−7.375469	0.000000
C	−2.887963	−8.579894	0.000000
H	−3.427870	−9.529057	0.000000
C	−3.576183	−7.398593	0.000000
C	−2.886387	−6.138619	0.000000
H	−4.667985	−7.396632	0.000000

[a] Final energy (in a.u.): -1839.041556507.

Table S13: XYZ coordinates (in Å) for the fully optimized structure of circumbenzene at the B2-PLYP level[a]

C	1.419833	0.000000	0.000000
C	−1.419833	0.000000	0.000000
C	0.709258	−1.234895	0.000000
C	−0.709258	1.234895	0.000000
C	0.709258	1.234895	0.000000
C	−0.709258	−1.234895	0.000000
C	1.426376	−2.476208	0.000000
C	−1.426377	2.476208	0.000000
C	1.426376	2.476208	0.000000
C	−1.426376	−2.476208	0.000000
C	0.684544	−3.707821	0.000000
C	−0.684544	3.707821	0.000000
C	0.684544	3.707821	0.000000
C	−0.684544	−3.707821	0.000000
C	2.840045	0.000000	0.000000
C	−2.840045	0.000000	0.000000
C	3.527543	−1.244259	0.000000
C	−3.527543	1.244259	0.000000
C	3.527543	1.244259	0.000000
C	−3.527543	−1.244259	0.000000
C	2.837946	−2.450146	0.000000
C	−2.837947	2.450146	0.000000
C	2.837946	2.450146	0.000000
C	−2.837946	−2.450146	0.000000
H	4.619248	−1.244778	0.000000
H	−4.619248	1.244778	0.000000
H	4.619248	1.244778	0.000000
H	−4.619248	−1.244777	0.000000
H	3.389376	−3.391398	0.000000
H	−3.389377	3.391398	0.000000
H	3.389376	3.391398	0.000000
H	−3.389377	−3.391398	0.000000
H	1.235959	−4.649167	0.000000
H	−1.235960	4.649166	0.000000
H	1.235959	4.649167	0.000000
H	−1.235960	−4.649166	0.000000

[a] Final energy (in a.u.): -920.997866174.

Table S14: XYZ coordinates (in Å) for the fully optimized structure of circumnaphtalene at the B2-PLYP level[a]

C	−0.711916	0.000000	0.000000
C	−1.422464	1.233760	0.000000
C	−0.712584	2.465799	0.000000
C	−1.427088	3.700754	0.000000
C	−0.688094	4.923638	0.000000
C	−2.851053	3.675446	0.000000
C	−3.541319	2.482848	0.000000
C	−2.851177	1.231858	0.000000
C	−3.534747	0.000000	0.000000
C	−2.851177	−1.231858	0.000000
C	−3.541319	−2.482847	0.000000
C	−2.851053	−3.675446	0.000000
C	−1.427087	−3.700754	0.000000
C	−1.422464	−1.233760	0.000000
C	−0.688094	−4.923638	0.000000
C	−0.712584	−2.465799	0.000000
C	0.688093	−4.923638	0.000000
C	0.712585	−2.465799	0.000000
C	0.711917	0.000000	0.000000
C	0.712585	2.465799	0.000000
C	0.688093	4.923638	0.000000
C	1.427087	−3.700754	0.000000
C	1.422465	−1.233760	0.000000
C	1.422464	1.233760	0.000000
C	1.427087	3.700754	0.000000
C	2.851053	−3.675446	0.000000
C	2.851178	−1.231858	0.000000
C	2.851178	1.231858	0.000000
C	2.851053	3.675447	0.000000
C	3.541319	−2.482848	0.000000
C	3.534748	0.000000	0.000000
C	3.541319	2.482848	0.000000
H	−4.627559	0.000000	0.000000
H	−4.632712	2.482466	0.000000
H	−4.632712	−2.482466	0.000000
H	−3.395414	4.621040	0.000000
H	−3.395413	−4.621040	0.000000
H	−1.235597	5.867520	0.000000
H	−1.235597	−5.867520	0.000000
H	1.235595	−5.867520	0.000000
H	3.395413	−4.621040	0.000000
H	4.632712	−2.482467	0.000000
H	4.627560	0.000000	0.000000
H	4.632712	2.482467	0.000000
H	3.395413	4.621040	0.000000
H	1.235596	5.867520	0.000000

[a] Final energy (in a.u.): -1226.932565382.

Table S15: XYZ coordinates (in Å) for the fully optimized structure of circumanthracene at the B2-PLYP level[a]

C	3.545267	2.482729	0.000000
C	2.855013	1.226135	0.000000
C	1.420935	1.228548	0.000000
C	0.710704	2.460618	0.000000
C	1.424767	3.694119	0.000000
C	2.855281	3.668610	0.000000
C	0.708482	−0.003239	0.000000
C	−0.719668	−0.002064	0.000000
C	−1.430091	1.230879	0.000000
C	−0.717806	2.461777	0.000000
C	−2.864177	1.230850	0.000000
C	−3.548144	0.006700	0.000000
C	−2.863675	−1.229943	0.000000
C	−1.427702	−1.231135	0.000000
C	1.414490	−1.233461	0.000000
C	0.706456	−2.462533	0.000000
C	−0.721694	−2.461358	0.000000
C	−3.552372	2.488565	0.000000
C	−2.860378	3.673282	0.000000
C	−1.429834	3.696422	0.000000
C	0.689116	4.911056	0.000000
C	−0.692182	4.912137	0.000000
C	−1.434146	−3.693144	0.000000
C	−2.868224	−3.690733	0.000000
C	−3.550168	−2.465497	0.000000
C	1.416879	−3.695475	0.000000
C	0.704594	−4.926375	0.000000
C	−0.723916	−4.925215	0.000000
C	2.850463	−1.234654	0.000000
C	3.534933	−2.471298	0.000000
C	2.850965	−3.695448	0.000000
C	3.536957	0.000899	0.000000
H	−4.640847	0.007292	0.000000
H	−4.643670	2.489234	0.000000
H	−4.642871	−2.464284	0.000000
H	−3.399567	4.621969	0.000000
H	−1.236645	5.857948	0.000000
C	−1.437982	−6.158714	0.000000
C	1.416622	−6.161019	0.000000
H	4.627635	−2.471888	0.000000
H	4.629660	−0.000311	0.000000
H	4.636567	2.481576	0.000000
H	3.396065	4.616387	0.000000
H	1.235100	5.855987	0.000000
C	2.847168	−6.137879	0.000000
C	0.678968	−7.376732	0.000000
H	3.386348	−7.086571	0.000000
C	3.539160	−4.953162	0.000000
H	4.630458	−4.953828	0.000000
C	−0.702331	−7.375649	0.000000
C	−2.868497	−6.133207	0.000000
H	−1.248304	−8.320587	0.000000
H	1.223419	−8.322550	0.000000
C	−3.558481	−4.947326	0.000000
H	−3.409269	−7.080991	0.000000
H	−4.649781	−4.946162	0.000000

[a] Final energy (in a.u.): -1532.853631456.

Table S16: XYZ coordinates (in Å) for the fully optimized structure of circumtetracene at the B2-PLYP level[a]

C	−3.566960	−4.915572	0.000000
C	−2.877233	−3.678929	0.000000
C	−1.437248	−3.681832	0.000000
C	−0.733882	−4.911317	0.000000
C	−1.449051	−6.141071	0.000000
C	−3.558566	−2.445189	0.000000
C	−2.870416	−1.215243	0.000000
C	−1.430433	−1.220310	0.000000
C	−0.725650	−2.453031	0.000000
C	−0.720259	0.005248	0.000000
C	−1.428587	1.238946	0.000000
C	−2.865995	1.242858	0.000000
C	−3.553250	0.025219	0.000000
C	−0.712481	2.468258	0.000000
C	0.717717	2.464292	0.000000
C	1.426994	1.231029	0.000000
C	0.711837	0.001277	0.000000
C	1.433183	3.697326	0.000000
C	2.866921	3.669568	0.000000
C	3.555628	2.486868	0.000000
C	2.864400	1.226970	0.000000
C	1.415204	−1.228199	0.000000
C	2.855194	−1.231121	0.000000
C	3.544892	0.005537	0.000000
C	−1.421098	3.705240	0.000000
C	−0.682795	4.915322	0.000000
C	0.701601	4.911484	0.000000
C	0.703587	−2.456990	0.000000
C	−3.550226	2.506571	0.000000
C	−2.854969	3.685432	0.000000
C	3.536524	−2.464862	0.000000
C	2.848357	−3.694799	0.000000
C	1.408373	−3.689704	0.000000
C	0.698216	−4.915278	0.000000
C	3.531186	−4.935264	0.000000
C	2.843943	−6.152913	0.000000
C	1.406541	−6.148973	0.000000
C	0.690422	−7.378295	0.000000
H	−4.645828	0.028232	0.000000
H	−4.641538	2.509812	0.000000
H	−4.651356	−2.442114	0.000000
H	−3.389233	4.637068	0.000000
H	−1.224098	5.863095	0.000000
H	4.629314	−2.467841	0.000000
H	4.637470	0.002495	0.000000
H	4.646941	2.484053	0.000000
H	3.406454	4.618227	0.000000
H	1.248152	5.856240	0.000000
H	4.623765	−4.938172	0.000000
C	1.399073	−8.615263	0.000000
H	−4.659534	−4.912456	0.000000
C	0.660769	−9.825340	0.000000
C	2.832936	−8.595465	0.000000
H	1.201983	−10.773164	0.000000
C	−0.723635	−9.821502	0.000000
H	−1.270138	−10.766287	0.000000
C	−1.455241	−8.607367	0.000000
C	3.528205	−7.416603	0.000000
H	3.367206	−9.547098	0.000000
H	4.619514	−7.419874	0.000000
C	−0.739758	−7.374320	0.000000
C	−2.888950	−8.579583	0.000000
H	−3.428590	−9.528184	0.000000
C	−3.577692	−7.396880	0.000000
C	−2.886455	−6.136999	0.000000
H	−4.669002	−7.394221	0.000000

[a] Final energy (in a.u.): -1838.767085137.