–Supporting Information–

The Role of Topology in Organic Molecules: Origin and Comparison of the Radical Character in Linear and Cyclic Oligoacenes and Related Oligomers

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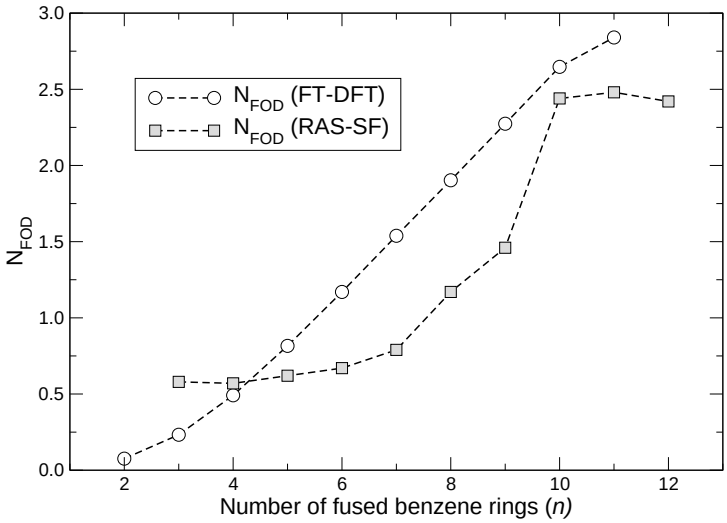

Figure 1: Evolution of the N_{FOD} values for oligoacenes as a function of the system size.

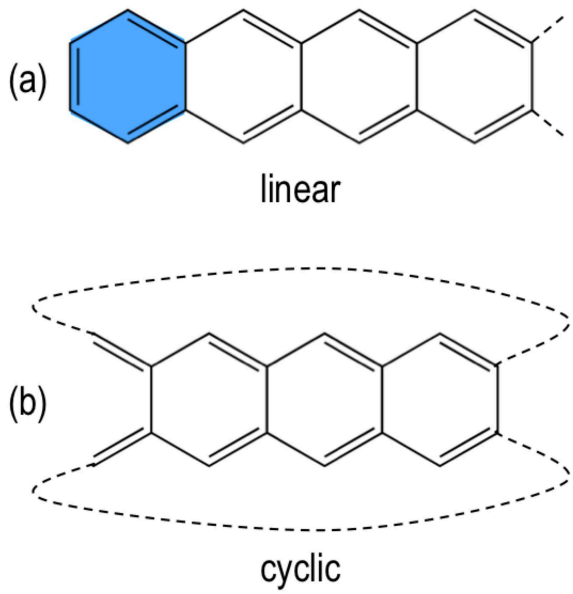

Figure 2: Resonance structures for linear (a) and cyclic (b) acenes. Clar's sexted ring indicated in blue.

1 The symmetrized von Neumann entropy

The f_i occupation numbers obtained from the FT-TPSS calculations (or the RAS-SF occupation numbers by using $f_i = n_i/2$) can also be used to calculate the symmetrized von Neumann entropy:

$$\mathcal{S} = -\frac{1}{2}\sum_{i}^{\infty}\left[f_i \ln\left(f_i\right) + \left(1-f_i\right)\ln\left(1-f_i\right)\right], \tag{1}$$

with $\mathcal{S} = 0$ for a system having associated an idempotent one-particle density matrix (i.e. f_i equal to 0 or 1) or, in other words, for pure states. Deviations from this limit should be interpreted as entangled states,[1] needing thus more than one Slater determinant[2] for their adequate description, which would result in another proof of its polyradicaloid nature. Figure 3 shows the large and growing entropy per carbon atom in the case of linear oligoacenes, as it also happened for graphene nanoribbons,[3] and how the odd-even trend is preserved in the case of [n]CC molecules. Note also that values seems to saturate for the largest compounds studied here in both cases. These results are fully consistent with a polyradicaloid nature.

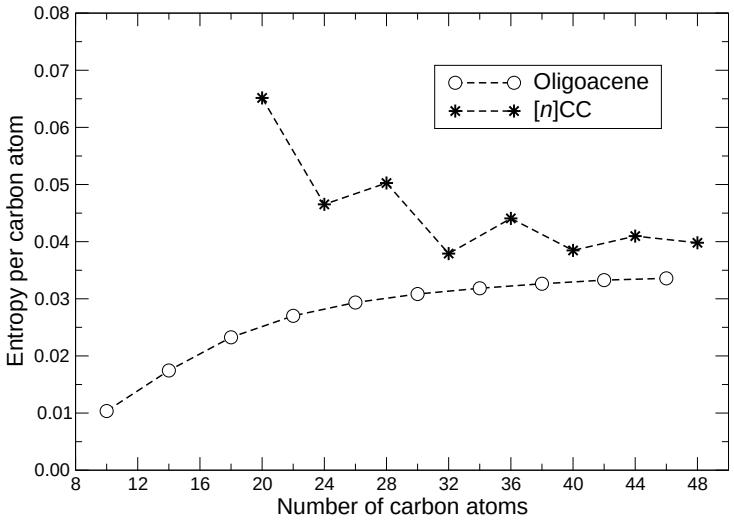

Figure 3: Evolution of the entropy per carbon as a function of the total number of carbon atoms.

2 A qualitative Hückel-based measure of the radicaloid character

A simple estimate of the atom-centered radicaloid character for the non-bridging C atoms in linear and cyclic oligoacenes can be obtained by the following approach:

$$C_i = p_{ij}(\text{benzene}) - p_{ij}(\text{oligoacene}), \tag{2}$$

with p_{ij} the bond orders between atoms i and j, and taking the isolated benzene unit as reference, with all structures optimized at the M06-2X/6-31+G* level. The previous expression can be seen as a generalization of Coulson's free valence index,[4,5] which roughly correlates with the reactivity of an atom in a molecule against a free radical attack. The total radicaloid character of a molecule is obtained as $C_t = \sum_i C_i$. Figure 4 shows the evolution of this radicaloid character, increasing as a function of the total number of fused rings, and Figure 5 presents how the average C_i values tends to saturate for

the largest compounds.

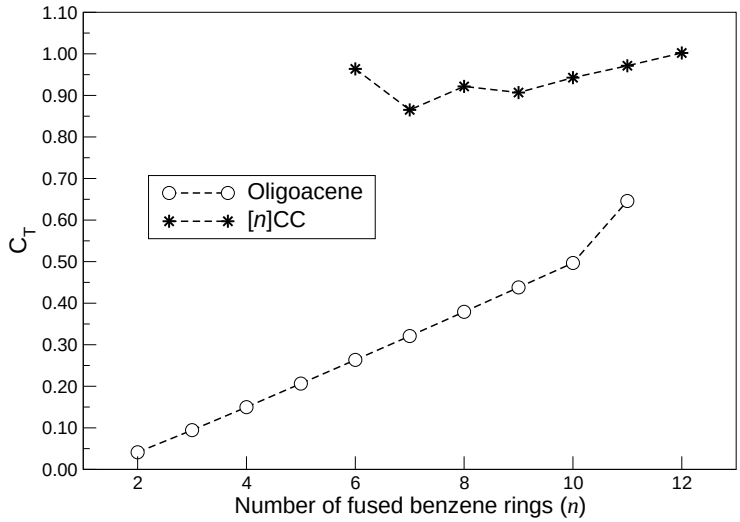

Figure 4: Evolution of total C_i values, as a function of the oligomer size for both linear and cyclic acenes.

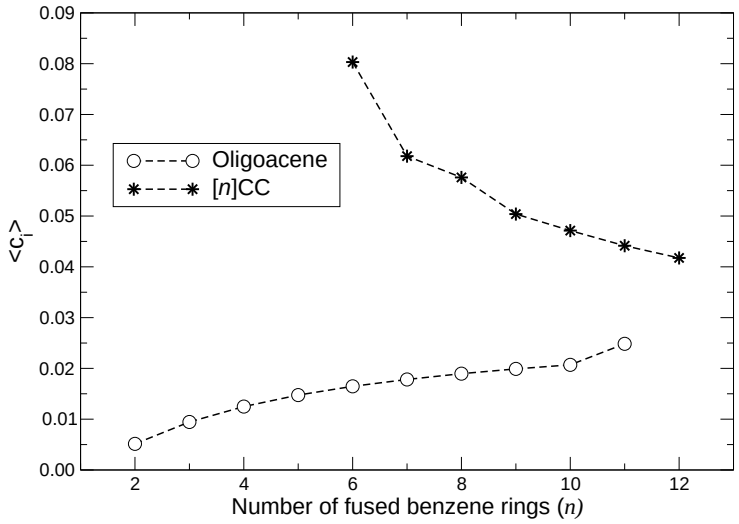

Figure 5: Evolution of averaged C_i values, as a function of the oligomer size for both linear and cyclic acenes.

3 Relationship between N_{FOD} values and HOMO-LUMO energy difference

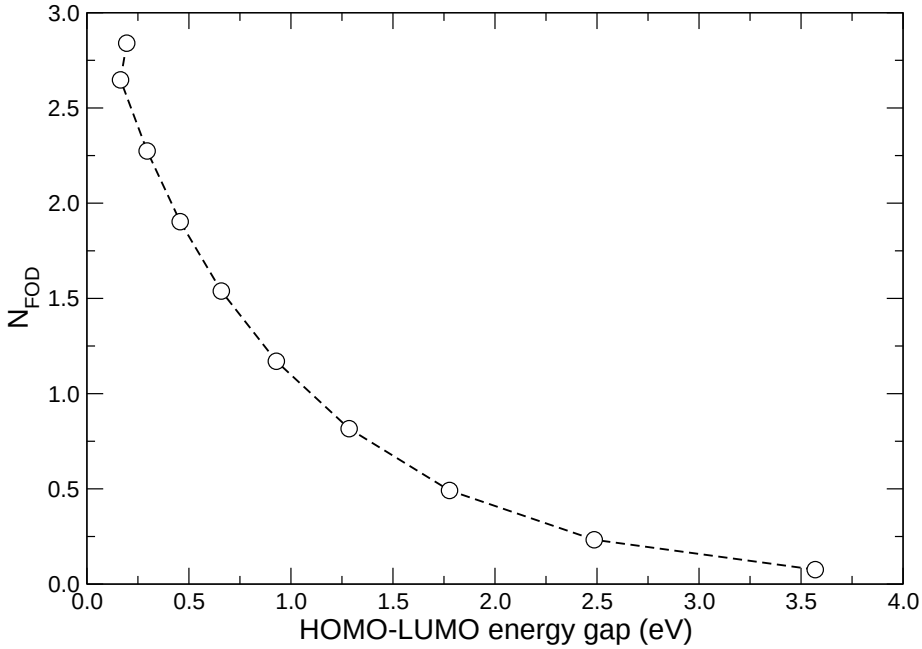

Figure 6: Relationship between N_{FOD} values and HOMO-LUMO energy difference

4 Relationship between y (biradical character) and N_{FOD} values

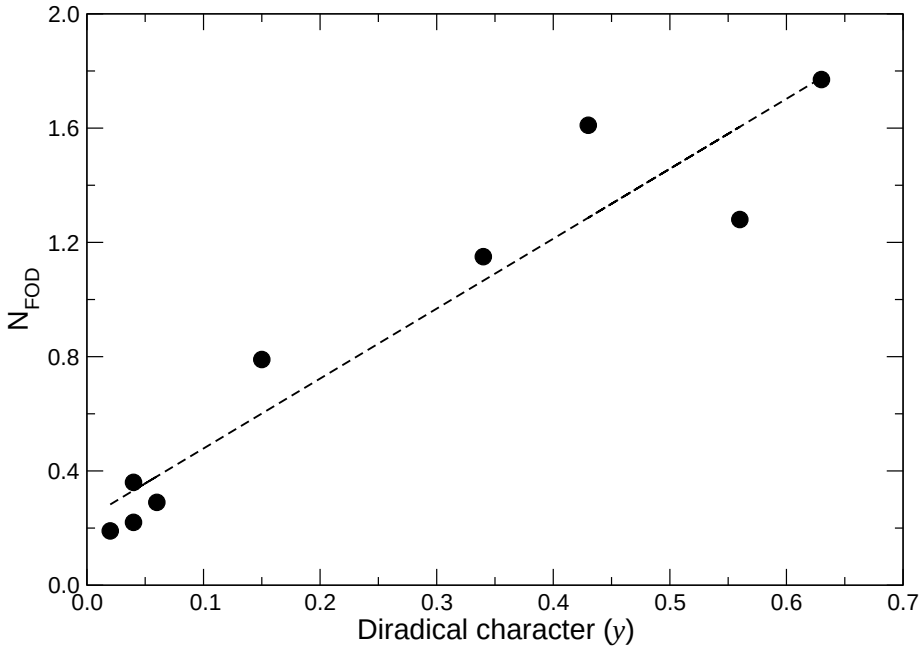

Figure 7: Relationship between y (biradical character) and N_{FOD} values

5 Additional information from FT-TPSS calculations

Table S1: Energy and orbitals occupation (spin up) at the TPSS/def2-TZVP (T_{el} = 5000K) level, and N_{FOD} values, for [n]CPPs of increasing size.

	[5]CPP		[6]CPP		[7]CPP		[8]CPP	
	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.
(L+4)UMO	–1.4369	0.0058	–1.2594	0.0037	–1.3590	0.0045	–1.2675	0.0037
(L+3)UMO	–1.5368	0.0073	–1.4651	0.0060	–1.4863	0.0061	–1.3512	0.0044
(L+2)UMO	–1.6479	0.0094	–1.8044	0.0130	–1.8706	0.0147	–1.9905	0.0193
(L+1)UMO	–1.6788	0.0101	–1.8055	0.0131	–1.9765	0.0187	–1.9906	0.0193
LUMO	–2.7586	0.1109	–2.5594	0.0707	–2.5602	0.0686	–2.4535	0.0544
HOMO	–4.5122	0.8796	–4.7419	0.9234	–4.7823	0.9275	–4.8945	0.9432
(H-1)OMO	–5.6655	0.9907	–5.5036	0.9860	–5.3590	0.9799	–5.3362	0.9789
(H-2)OMO	–5.6845	0.9911	–5.5046	0.9861	–5.4432	0.9834	–5.3362	0.9789
(H-3)OMO	–6.1641	0.9970	–6.2602	0.9976	–6.2395	0.9974	–6.1823	0.9970
(H-4)OMO	–6.2394	0.9975	–6.3475	0.9980	–6.3073	0.9977	–6.1831	0.9970
N_{FOD}	0.59498		0.46873		0.50452		0.48338	

Table S1 (cont.): Energy and orbitals occupation (spin up) at the TPSS/def2-TZVP ($T_{el} = 5000$K) level, and N_{FOD} values, for [n]CPPs of increasing size.

	[9]CPP		[10]CPP		[11]CPP		[12]CPP	
	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.
(L+4)UMO	–1.4246	0.0051	–1.4341	0.0052	–1.5085	0.0062	–1.6045	0.0077
(L+3)UMO	–1.4562	0.0055	–1.4745	0.0057	–1.5849	0.0074	–1.6756	0.0091
(L+2)UMO	–2.0451	0.0212	–2.0733	0.0226	–2.1164	0.0249	–2.1584	0.0273
(L+1)UMO	–2.1481	0.0268	–2.1826	0.0289	–2.1652	0.0279	–0.9765	0.0187
LUMO	–2.5201	0.0642	–2.4615	0.0538	–2.4125	0.0484	–2.4125	0.0482
HOMO	–4.8573	0.9367	–4.9226	0.9450	–4.9732	0.9510	–4.9793	0.9514
(H-1)OMO	–5.2190	0.9690	–5.1895	0.9696	–5.2025	0.9706	–5.1731	0.9684
(H-2)OMO	–5.3026	0.9765	–5.2796	0.9752	–5.2436	0.9732	–5.2131	0.9712
(H-3)OMO	–5.9914	0.9952	–5.8723	0.9936	–5.7416	0.9914	–5.6587	0.9896
(H-4)OMO	–6.1036	0.9963	–5.9224	0.9943	–5.8122	0.9927	–5.7212	0.9909
N_{FOD}	0.57201		0.57873		0.58906		0.63630	

Table S2: Energy and orbitals occupation (spin up) at the TPSS/def2-TZVP (T_{el} = 5000K) level, and N_{FOD} values, for linear oligoacenes of increasing size.

	Naphtalene		Anthracene		Tetracene		Pentacene		Hexacene	
	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.
(L+4)UMO	1.3732	0.0000	0.7146	0.0000	–0.1129	0.0002	–0.2431	0.0003	–0.4847	0.0005
(L+3)UMO	1.0247	0.0000	–0.1525	0.0003	–0.4154	0.0005	–0.7944	0.0011	–1.1784	0.0025
(L+2)UMO	–0.3018	0.0004	–0.8374	0.0013	–1.2605	0.0033	–1.2971	0.0034	–1.3222	0.0035
(L+1)UMO	–1.1203	0.0028	–1.2058	0.0031	–1.3824	0.0044	–1.8322	0.0118	–2.1885	0.0259
LUMO	–1.8683	0.0157	–2.4521	0.0534	–2.8382	0.1143	–3.1063	0.1868	–3.2996	0.2593
HOMO	–5.4380	0.9844	–4.9386	0.9476	–4.6155	0.8886	–4.3915	0.8194	–4.2282	0.7513
(H-1)OMO	–6.1564	0.9970	–6.1078	0.9963	–5.9101	0.9938	–5.5135	0.9840	–5.2076	0.9670
(H-2)OMO	–7.1099	0.9997	–6.4339	0.9983	–6.0820	0.9958	–6.0667	0.9955	–6.0572	0.9953
(H-3)OMO	–8.0231	1.0000	–7.4543	0.9998	–6.9509	0.9994	–6.4974	0.9983	–6.1161	0.9959
(H-4)OMO	–8.1599	1.0000	–7.6074	0.9999	–7.2485	0.9997	–7.0006	0.9995	–6.8218	0.9992
N_{FOD}	0.07589		0.23260		0.49137		0.81609		1.17000	

Table S2 (cont.): Energy and orbitals occupation (spin up) at the TPSS/def2-TZVP (T_{el} = 5000K) level, and N_{FOD} values, for linear oligoacenes of increasing size.

	Heptacene		Octacene		Nonacene		Decacene		Undecacene	
	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.
(L+4)UMO	–0.7751	0.0010	–1.0698	0.0019	–1.3463	0.0036	–1.3797	0.0038	–1.3493	0.0035
(L+3)UMO	–1.3424	0.0036	–1.3579	0.0037	–1.3700	0.0038	–1.5969	0.0063	–1.8458	0.0109
(L+2)UMO	–1.5242	0.0055	–1.8229	0.0109	–2.0778	0.0193	–2.2950	0.0312	–2.5095	0.0490
(L+1)UMO	–2.4709	0.0477	–2.6966	0.0777	–2.8801	0.1123	–3.0312	0.1511	–3.1418	0.1827
LUMO	–3.4462	0.3252	–3.5555	0.3799	–3.6432	0.4263	–3.7137	0.4646	–3.7125	0.4567
HOMO	–4.1051	0.6899	–4.0128	0.6391	–3.9384	0.5958	–3.8786	0.5599	–3.9079	0.5695
(H-1)OMO	–4.9692	0.9429	–4.7785	0.9128	–4.6230	0.8784	–4.4946	0.8416	–4.4230	0.8139
(H-2)OMO	–5.8021	0.9913	–5.5412	0.9840	–5.3227	0.9734	–5.1379	0.9594	–4.9701	0.9396
(H-3)OMO	–6.0504	0.9951	–6.0450	0.9950	–5.9739	0.9940	–5.7501	0.9899	–5.5465	0.9834
(H-4)OMO	–6.5289	0.9984	–6.2319	0.9967	–6.0416	0.9949	–6.0393	0.9948	–6.0720	0.9950
N_{FOD}	1.53838		1.90275		2.27394		2.64724		2.84002	

Table S3: Energy and orbitals occupation (spin up) at the TPSS/def2-TZVP (T_{el} = 5000K) level, and N_{FOD} values, for cyclic oligoacenes of increasing size.

	[5]CC		[6]CC		[7]CC		[8]CC	
	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.
(L+4)UMO	–2.0087	0.0174	–1.7901	0.0134	–1.4847	0.0072	–1.3043	0.0043
(L+3)UMO	–2.0128	0.0176	–1.9851	0.0210	–1.4973	0.0074	–1.7651	0.0123
(L+2)UMO	–2.6780	0.0774	–1.9942	0.0214	–2.1508	0.0329	–2.4626	0.0591
(L+1)UMO	–2.6800	0.3777	–2.7754	0.1182	–3.1988	0.2793	–2.4626	0.0591
LUMO	–3.5068	0.3647	–3.1715	0.2515	–3.2000	0.2799	–3.3120	0.3110
HOMO	–4.1616	0.7241	–3.8368	0.6115	–3.9584	0.6932	–3.9652	0.6728
(H-1)OMO	–4.1649	0.7256	–5.3055	0.9794	–3.9602	0.6941	–4.8287	0.9385
(H-2)OMO	–6.3638	0.9977	–5.3109	0.9797	–6.1243	0.9971	–4.8288	0.9385
(H-3)OMO	–6.3638	0.9977	–5.5496	0.9882	–6.1254	0.9971	–5.7636	0.9926
(H-4)OMO	–7.0402	0.9995	–7.3650	0.9998	–6.3208	0.9982	–6.5698	0.9988
N_{FOD}	2.23588		1.76764		2.48990		1.84347	

Table S3 (cont.): Energy and orbitals occupation (spin up) at the TPSS/def2-TZVP (T_{el} = 5000K) level, and N_{FOD} values, for cyclic oligoacenes of increasing size.

	[9]CC		[10]CC		[11]CC		[12]CC	
	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.
(L+4)UMO	–1.4410	0.0055	–1.4496	0.0053	–1.1569	0.0026	–1.8811	0.0123
(L+3)UMO	–1.8653	0.0147	–1.4523	0.0053	–2.3006	0.0353	–1.8831	0.0125
(L+2)UMO	–1.8700	0.0148	–2.8696	0.1259	–2.3025	0.0354	–3.1834	0.2085
(L+1)UMO	–3.5159	0.4068	–2.8702	0.1260	–3.7058	0.4883	–3.1834	0.2086
LUMO	–3.5167	0.4072	–3.3874	0.3238	–3.7086	0.4899	–3.4344	0.3281
HOMO	–3.8284	0.5861	–4.0361	0.6834	–3.7483	0.5130	–4.0821	0.6858
(H-1)OMO	–3.8303	0.5872	–4.5136	0.8673	–3.7490	0.5134	–4.2909	0.7859
(H-2)OMO	–5.5141	0.9861	–4.5156	0.8679	–5.0999	0.9604	–4.2909	0.7859
(H-3)OMO	–5.5166	0.9862	–5.8607	0.9933	–5.1022	0.9606	–5.5333	0.9852
(H-4)OMO	–6.2544	0.9975	–5.9852	0.9950	–6.2068	0.9969	–5.5376	0.9855
N_{FOD}	3.44412		2.40120		4.25839		3.13283	

Table S4: Energy and orbitals occupation (spin up) at the TPSS/def2-TZVP (T_{el} = 5000K) level, and N_{FOD} values, for other nanorings.

	Cyclo[a]decacene		Cyclo[a]undecacene		[3]Cyclobenzo[a]anthracene		[3]Cyclochrysene	
	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.	E(ev)	Occ.
(L+4)UMO	–1.4688	0.0060	–1.4734	0.0058	–1.9314	0.0161	–1.9110	0.0168
(L+3)UMO	–1.7330	0.0109	–1.9703	0.0182	–2.0301	0.0202	–1.9995	0.0205
(L+2)UMO	–2.4015	0.0496	–2.1981	0.0306	–2.0309	0.0203	–2.0046	0.0207
(L+1)UMO	–2.7240	0.0994	–3.1600	0.2272	–2.3640	0.0429	–2.0821	0.0247
LUMO	–3.6177	0.4675	–3.5557	0.4241	–2.7833	0.1060	–2.7304	0.1025
HOMO	–3.7215	0.5277	–3.8322	0.5832	–4.6903	0.9083	–4.6827	0.9138
(H-1)OMO	–4.6296	0.9019	–4.1843	0.7601	–4.9059	0.9423	–5.0838	0.9641
(H-2)OMO	–4.8866	0.9435	–5.1985	0.9709	–5.2830	0.9751	–5.2846	0.9772
(H-3)OMO	–5.6333	0.9895	–5.3773	0.9806	–5.2856	0.9753	–5.2864	0.9773
(H-4)OMO	–6.0233	0.9957	–5.9230	0.9944	–5.6114	0.9882	–5.3432	0.9800
N_{FOD}	2.59213		2.88054		0.92915		0.88088	

6 Additional information from RAS-SF calculations

Table S5: Natural orbital occupation (spin up and down) at the RAS-SF/6-31G(d) level, and N_{FOD} values, for linear oligoacenes of increasing size.

	Anthracene	Tetracene	Pentacene	Hexacene	Heptacene
(L+3)UNO	0.045	0.037	0.040	0.035	0.033
(L+2)UNO	0.054	0.047	0.041	0.038	0.044
(L+1)UNO	0.058	0.059	0.054	0.064	0.068
LUNO	0.118	0.117	0.157	0.175	0.229
HONO	1.883	1.884	1.844	1.826	1.772
(H-1)ONO	1.941	1.940	1.946	1.936	1.932
(H-2)ONO	1.946	1.952	1.958	1.961	1.955
(H-3)ONO	1.953	1.961	1.959	1.964	1.966
N_{FOD}	0.58	0.57	0.62	0.67	0.79

Table S5 (cont.): Natural orbital occupation (spin up and down) at the RAS-SF/6-31G(d) level, and N_{FOD} values, for linear oligoacenes of increasing size.

	Octacene	Nonacene	Decacene	Undecacene	Dodecacene
(L+3)UNO	0.028	0.024	0.036	0.037	0.042
(L+2)UNO	0.046	0.055	0.063	0.069	0.072
(L+1)UNO	0.084	0.090	0.122	0.124	0.133
LUNO	0.403	0.538	0.982	0.988	0.943
HONO	1.598	1.462	1.018	1.013	1.058
(H-1)ONO	1.916	1.910	1.879	1.876	1.867
(H-2)ONO	1.953	1.945	1.937	1.930	1.927
(H-3)ONO	1.971	1.975	1.963	1.962	1.957
N_{FOD}	1.17	1.46	2.44	2.48	2.42

Table S6: Natural orbital occupation (spin up and down) at the RAS-SF/6-31G(d) level, and N_{FOD} values, for cyclic oligoacenes of increasing size.

	[5]CC	[6]CC	[7]CC	[8]CC	[9]CC	[10]CC	[11]CC	[12]CC[a]
(L+3)UNO	0.029	0.024	0.066	0.039	0.080	0.034	0.096	0.027
(L+2)UNO	0.044	0.101	0.066	0.119	0.082	0.135	0.102	0.186
(L+1)UNO	0.216	0.102	0.368	0.119	0.549	0.158	0.682	0.186
LUNO	0.266	0.542	0.369	0.542	0.549	0.570	0.689	0.664
HONO	1.731	1.457	1.626	1.462	1.449	1.435	1.310	1.340
(H-1)ONO	1.778	1.902	1.627	1.880	1.449	1.841	1.317	1.813
(H-2)ONO	1.955	1.902	1.935	1.880	1.918	1.864	1.898	1.813
(H-3)ONO	1.957	1.959	1.935	1.957	1.921	1.963	1.904	1.971
N_{FOD}	1.22	1.60	1.79	1.66	2.57	1.82	3.19	2.15

[a]RAS-SF calculations for [12]CC have been performed using the (U)M06-2X/6-31+G(d) optimized geometry.

7 Cartesian coordinadates of all relevant compounds

Table S7: Cartesian coordinates of naphtalene

C	1.594028	1.465619	0.000000
C	1.512814	2.881308	0.000000
C	2.656864	3.639358	0.000000
C	2.817286	0.843376	0.000000
C	4.019366	1.601547	0.000000
C	3.937787	3.023639	0.000000
H	2.599510	4.725437	0.000000
H	2.884515	-0.242136	0.000000
C	5.139841	3.781782	0.000000
C	5.300274	0.985858	0.000000
C	6.444345	1.743901	0.000000
C	6.363128	3.159564	0.000000
H	7.274487	3.750169	0.000000
H	5.072524	4.867292	0.000000
H	5.357551	-0.100229	0.000000
H	7.417293	1.261431	0.000000
H	0.539875	3.363795	0.000000
H	0.682654	0.875039	0.000000

Table S7 (cont.): Cartesian coordinates of anthracene

C	-0.792721	1.296495	0.000000
C	-0.881923	2.723004	0.000000
C	0.249314	3.486211	0.000000
C	0.424773	0.680148	0.000000
C	1.635896	1.444613	0.000000
C	1.546227	2.878566	0.000000
H	0.186443	4.571794	0.000000
H	0.497605	-0.404814	0.000000
C	2.721026	3.635779	0.000000
C	2.895871	0.839665	0.000000
C	4.070666	1.596871	0.000000
C	3.981005	3.030822	0.000000
H	2.653067	4.722380	0.000000
H	2.963826	-0.246940	0.000000
C	5.192116	3.795298	0.000000
C	5.367591	0.989240	0.000000
C	6.498821	1.752458	0.000000
C	6.409617	3.178969	0.000000
H	7.320768	3.769810	0.000000
H	5.119247	4.880257	0.000000
H	5.430484	-0.096343	0.000000
H	7.476489	1.279744	0.000000
H	-1.859582	3.195732	0.000000
H	-1.703895	0.705682	0.000000

Table S7 (cont.): Cartesian coordinates of tetracene

C	-3.284214	2.697712	0.000000
C	-2.145502	3.443136	0.000000
C	-3.216853	1.264155	0.000000
C	-2.013254	0.628844	0.000000
C	-0.783796	1.373611	0.000000
C	-0.851601	2.816969	0.000000
H	-2.191934	4.529521	0.000000
H	-1.957566	-0.457101	0.000000
C	0.323780	3.554400	0.000000
C	0.455582	0.749627	0.000000
C	1.656049	1.489019	0.000000
C	1.588286	2.930862	0.000000
H	0.273007	4.641853	0.000000
H	0.506964	-0.337792	0.000000
C	2.788743	3.670251	0.000000
C	2.920569	0.865480	0.000000
C	4.095957	1.602937	0.000000
C	4.028114	3.046296	0.000000
H	2.737351	4.757673	0.000000
H	2.971351	-0.221968	0.000000
C	5.257572	3.791070	0.000000
C	5.389856	0.976773	0.000000
C	6.528558	1.722190	0.000000
C	6.461183	3.155749	0.000000
H	7.382543	3.730465	0.000000
H	5.201896	4.877019	0.000000
H	5.436274	-0.109609	0.000000
H	7.499760	1.236425	0.000000
H	-4.255427	3.183465	0.000000
H	-4.138189	0.689410	0.000000

Table S7 (cont.): Cartesian coordinates of pentacene

C	-3.319508	2.686182	0.000000
C	-2.151481	3.425793	0.000000
C	-3.247885	1.238211	0.000000
C	-2.012605	0.617411	0.000000
C	-0.806165	1.359424	0.000000
C	-0.877727	2.806432	0.000000
H	-2.205197	4.513033	0.000000
H	-1.958807	-0.469827	0.000000
C	0.309525	3.547455	0.000000
C	0.448412	0.739153	0.000000
C	1.635442	1.480162	0.000000
C	1.563872	2.927193	0.000000
H	0.255724	4.634604	0.000000
H	0.502133	-0.348000	0.000000
C	2.770526	3.669230	0.000000
C	2.909434	0.860817	0.000000
C	4.077252	1.600442	0.000000
C	4.005629	3.048458	0.000000
H	2.716657	4.756469	0.000000
H	2.963110	-0.226431	0.000000
C	5.236864	3.795652	0.000000
C	5.376216	0.978399	0.000000
C	6.510870	1.726566	0.000000
C	6.439814	3.163111	0.000000
H	7.360366	3.739124	0.000000
H	5.178987	4.881453	0.000000
H	5.425771	-0.107813	0.000000
H	7.483774	1.244210	0.000000
C	-4.618403	3.308237	0.000000
C	-4.479076	0.491137	0.000000
C	-5.682141	1.123807	0.000000
C	-5.753044	2.560344	0.000000
H	-4.668135	4.394485	0.000000
H	-4.421427	-0.594731	0.000000
H	-6.725794	3.042951	0.000000
H	-6.602665	0.547794	0.000000

Table S7 (cont.): Cartesian coordinates of hexacene

C	-3.306428	2.665061	0.000000
C	-2.128317	3.409534	0.000000
C	-3.229573	1.214723	0.000000
C	-1.979379	0.598928	0.000000
C	-0.786694	1.344074	0.000000
C	-0.863560	2.794612	0.000000
H	-2.186039	4.496483	0.000000
H	-1.921902	-0.488033	0.000000
C	0.329125	3.539757	0.000000
C	0.478063	0.729152	0.000000
C	1.656175	1.473625	0.000000
C	1.579319	2.923964	0.000000
H	0.271648	4.626719	0.000000
H	0.535785	-0.357797	0.000000
C	2.787914	3.670060	0.000000
C	2.936854	0.859440	0.000000
C	4.098860	1.602897	0.000000
C	4.021986	3.053575	0.000000
H	2.730280	4.757117	0.000000
H	2.994429	-0.227620	0.000000
C	5.252598	3.804781	0.000000
C	5.401972	0.985957	0.000000
C	6.532685	1.738104	0.000000
C	6.456470	3.176348	0.000000
H	7.375424	3.754831	0.000000
H	5.190861	4.890369	0.000000
H	5.455313	-0.100075	0.000000
H	7.507630	1.259982	0.000000
C	-4.587107	3.279246	0.000000
C	-4.438168	0.468627	0.000000
C	-5.672240	1.085112	0.000000
C	-5.749113	2.535791	0.000000
H	-4.644682	4.366307	0.000000
H	-4.380534	-0.618430	0.000000
C	-7.052225	3.152731	0.000000
C	-6.902852	0.333907	0.000000
C	-8.106724	0.962340	0.000000
C	-8.182938	2.400585	0.000000
H	-9.157884	2.878707	0.000000
H	-7.105566	4.238763	0.000000
H	-6.841116	-0.751681	0.000000
H	-9.025678	0.383858	0.000000

Table S7 (cont.): Cartesian coordinates of heptacene

C	-3.478397	2.772597	0.000000
C	-2.276356	3.491075	0.000000
C	-3.432889	1.317928	0.000000
C	-2.188288	0.675983	0.000000
C	-0.986246	1.394468	0.000000
C	-1.031756	2.849137	0.000000
H	-2.310388	4.578970	0.000000
H	-2.154256	-0.411913	0.000000
C	0.181433	3.567923	0.000000
C	0.269523	0.752930	0.000000
C	1.460038	1.471371	0.000000
C	1.414544	2.925321	0.000000
H	0.148034	4.655860	0.000000
H	0.304180	-0.334968	0.000000
C	2.641300	3.644629	0.000000
C	2.729391	0.830176	0.000000
C	3.905684	1.548108	0.000000
C	3.860192	3.001655	0.000000
H	2.607997	4.732691	0.000000
H	2.764167	-0.257839	0.000000
C	5.107653	3.725673	0.000000
C	5.195988	0.903516	0.000000
C	6.342208	1.631044	0.000000
C	6.297128	3.071246	0.000000
H	7.228257	3.629978	0.000000
H	5.070183	4.812363	0.000000
H	5.226537	-0.183389	0.000000
H	7.306451	1.131629	0.000000
C	-4.734142	3.414144	0.000000
C	-4.646102	0.599149	0.000000
C	-5.879196	1.241771	0.000000
C	-5.924675	2.695721	0.000000
H	-4.768811	4.502041	0.000000
H	-4.612691	-0.488788	0.000000
C	-7.193991	3.336939	0.000000
C	-7.105988	0.522483	0.000000
C	-8.324856	1.165484	0.000000
C	-8.370310	2.619032	0.000000
H	-7.228769	4.424955	0.000000
H	-7.072685	-0.565577	0.000000
C	-9.660588	3.263656	0.000000
C	-9.572344	0.441495	0.000000
C	-10.761799	1.095951	0.000000
C	-10.806830	2.536154	0.000000
H	-11.771064	3.035589	0.000000
H	-9.691121	4.350562	0.000000
H	-9.534890	-0.645193	0.000000
H	-11.692938	0.537238	0.000000

Table S7 (cont.): Cartesian coordinates of octacene

C	-0.728526	2.448641	0.000000
C	-1.409011	1.228820	0.000000
C	0.728575	2.448647	0.000000
C	1.409076	1.228827	0.000000
C	0.728744	0.000000	0.000000
C	-0.728681	0.000000	0.000000
H	-2.497445	1.229053	0.000000
H	2.497507	1.229060	0.000000
C	-1.409011	-1.228820	0.000000
C	1.409076	-1.228827	0.000000
C	0.728575	-2.448647	0.000000
C	-0.728526	-2.448641	0.000000
H	-2.497445	-1.229053	0.000000
H	2.497507	-1.229060	0.000000
C	-1.408899	-3.687061	0.000000
C	1.408935	-3.687081	0.000000
C	0.728083	-4.896779	0.000000
C	-0.728073	-4.896767	0.000000
H	-2.497356	-3.687558	0.000000
H	2.497390	-3.687580	0.000000
C	-1.408643	-6.147606	0.000000
C	1.408631	-6.147632	0.000000
C	0.727793	-7.344210	0.000000
C	-0.727830	-7.344196	0.000000
H	-2.497216	-6.147735	0.000000
H	2.497202	-6.147769	0.000000
C	-1.408899	3.687061	0.000000
C	1.408935	3.687081	0.000000
C	0.728083	4.896779	0.000000
C	-0.728073	4.896767	0.000000
H	-2.497356	3.687558	0.000000
H	2.497390	3.687580	0.000000
C	-1.408643	6.147606	0.000000
C	1.408631	6.147632	0.000000
C	0.727794	7.344210	0.000000
C	-0.727830	7.344196	0.000000
H	-2.497216	6.147735	0.000000
H	2.497202	6.147769	0.000000
C	-1.412425	8.614829	0.000000
C	1.412367	8.614852	0.000000
C	0.721051	9.782497	0.000000
C	-0.721124	9.782488	0.000000
H	-1.249382	10.731178	0.000000
H	-2.499747	8.610638	0.000000
H	2.499688	8.610672	0.000000
H	1.249297	10.731191	0.000000
C	-1.412425	-8.614829	0.000000
C	1.412367	-8.614852	0.000000
C	0.721050	-9.782497	0.000000
C	-0.721124	-9.782488	0.000000
H	-1.249382	-10.731178	0.000000
H	-2.499747	-8.610638	0.000000
H	2.499688	-8.610672	0.000000
H	1.249297	-10.731191	0.000000

Table S7 (cont.): Cartesian coordinates of nonacene

C	-0.729496	1.224757	0.000000
C	-1.409678	0.000000	0.000000
C	0.729505	1.224757	0.000000
C	1.409688	0.000000	0.000000
C	0.729505	-1.224757	0.000000
C	-0.729496	-1.224757	0.000000
H	-2.498098	0.000000	0.000000
H	2.498108	0.000000	0.000000
C	-1.409574	-2.456714	0.000000
C	1.409582	-2.456716	0.000000
C	0.729173	-3.674049	0.000000
C	-0.729167	-3.674048	0.000000
H	-2.498002	-2.457163	0.000000
H	2.498010	-2.457165	0.000000
C	-1.409339	-4.914375	0.000000
C	1.409343	-4.914378	0.000000
C	0.728558	-6.122636	0.000000
C	-0.728558	-6.122634	0.000000
H	-2.497796	-4.915005	0.000000
H	2.497799	-4.915008	0.000000
C	-1.408964	-7.374553	0.000000
C	1.408961	-7.374557	0.000000
C	0.728166	-8.570387	0.000000
C	-0.728173	-8.570385	0.000000
H	-2.497541	-7.374729	0.000000
H	2.497538	-7.374733	0.000000
C	-1.409574	2.456714	0.000000
C	1.409582	2.456716	0.000000
C	0.729173	3.674049	0.000000
C	-0.729167	3.674048	0.000000
H	-2.498002	2.457163	0.000000
H	2.498010	2.457165	0.000000
C	-1.409340	4.914375	0.000000
C	1.409343	4.914378	0.000000
C	0.728558	6.122636	0.000000
C	-0.728558	6.122635	0.000000
H	-2.497796	4.915004	0.000000
H	2.497799	4.915008	0.000000
C	-1.408965	7.374553	0.000000
C	1.408961	7.374557	0.000000
C	0.728166	8.570387	0.000000
C	-0.728173	8.570385	0.000000
H	-2.497541	7.374729	0.000000
H	2.497537	7.374733	0.000000
C	-1.412649	-9.841535	0.000000
C	1.412640	-9.841538	0.000000
C	0.721335	-11.008870	0.000000
C	-0.721346	-11.008869	0.000000
H	-1.249382	-11.957675	0.000000
H	-2.499970	-9.837275	0.000000
H	2.499961	-9.837279	0.000000
H	1.249370	-11.957676	0.000000
C	-1.412650	9.841535	0.000000
C	1.412640	9.841538	0.000000
C	0.721335	11.008870	0.000000
C	-0.721347	11.008869	0.000000
H	-1.249382	11.957674	0.000000
H	-2.499970	9.837275	0.000000
H	2.499960	9.837279	0.000000
H	1.249369	11.957676	0.000000

Table S7 (cont.): Cartesian coordinates of decacene

C	0.729952	2.450099	0.000000
C	1.410073	1.227891	0.000000
C	-0.730060	2.450106	0.000000
C	-1.410199	1.227900	0.000000
C	-0.730236	0.000000	0.000000
C	0.730111	0.000000	0.000000
H	2.498480	1.228116	0.000000
H	-2.498607	1.228126	0.000000
C	1.410073	-1.227891	0.000000
C	-1.410199	-1.227901	0.000000
C	-0.730060	-2.450106	0.000000
C	0.729953	-2.450098	0.000000
H	2.498480	-1.228114	0.000000
H	-2.498607	-1.228129	0.000000
C	1.409888	-3.684022	0.000000
C	-1.409979	-3.684050	0.000000
C	-0.729585	-4.899801	0.000000
C	0.729529	-4.899786	0.000000
H	2.498312	-3.684621	0.000000
H	-2.498402	-3.684660	0.000000
C	1.409604	-6.141322	0.000000
C	-1.409629	-6.141361	0.000000
C	-0.728842	-7.348670	0.000000
C	0.728861	-7.348650	0.000000
H	2.498057	-6.142012	0.000000
H	-2.498081	-6.142070	0.000000
C	1.409887	3.684023	0.000000
C	-1.409979	3.684049	0.000000
C	-0.729586	4.899801	0.000000
C	0.729527	4.899787	0.000000
H	2.498311	3.684623	0.000000
H	-2.498403	3.684658	0.000000
C	1.409602	6.141324	0.000000
C	-1.409631	6.141359	0.000000
C	-0.728846	7.348669	0.000000
C	0.728857	7.348651	0.000000
H	2.498055	6.142015	0.000000
H	-2.498084	6.142068	0.000000
C	1.409209	8.601263	0.000000
C	-1.409161	8.601303	0.000000
C	-0.728354	9.796621	0.000000
C	0.728439	9.796602	0.000000
H	2.497783	8.601385	0.000000
H	-2.497735	8.601449	0.000000
C	1.409215	-8.601261	0.000000
C	-1.409155	-8.601305	0.000000
C	-0.728346	-9.796623	0.000000
C	0.728447	-9.796600	0.000000
H	2.497789	-8.601381	0.000000
H	-2.497729	-8.601452	0.000000
C	1.412880	11.068074	0.000000
C	-1.412760	11.068110	0.000000
C	-0.721438	12.235219	0.000000
C	0.721585	12.235203	0.000000
H	1.249423	13.184109	0.000000
H	2.500198	11.063709	0.000000
H	-2.500078	11.063770	0.000000
H	-1.249255	13.184136	0.000000
C	1.412890	-11.068071	0.000000
C	-1.412750	-11.068113	0.000000
C	-0.721425	-12.235220	0.000000
C	0.721598	-12.235202	0.000000
H	1.249437	-13.184107	0.000000
H	2.500208	-11.063705	0.000000
H	-2.500068	-11.063774	0.000000
H	-1.249241	-13.184138	0.000000

Table S7 (cont.): Cartesian coordinates of undecacene

C	-0.73492	0.00000	1.23864
C	-1.40534	0.00000	2.44785
H	-2.49432	0.00000	2.44881
C	-1.40347	0.00000	-0.00001
H	-2.49253	0.00000	-0.00000
C	-0.73493	0.00000	-1.23862
C	-1.40533	0.00000	-2.44786
H	-2.49432	0.00000	-2.44881
C	-0.73148	0.00000	-3.70924
C	-1.40665	0.00000	-4.90455
H	-2.49551	0.00000	-4.90607
C	-0.72620	0.00000	-6.16743
C	-1.40473	0.00000	-7.36888
H	-2.49354	0.00000	-7.37032
C	-0.72115	0.00000	-8.61531
C	-1.40220	0.00000	-9.83776
H	-2.49108	0.00000	-9.83828
C	-0.71906	0.00000	-11.05722
C	-0.73148	0.00000	3.70925
C	-1.40665	0.00000	4.90455
H	-2.49551	0.00000	4.90607
C	-0.72619	0.00000	6.16743
C	-1.40473	0.00000	7.36889
H	-2.49354	0.00000	7.37032
C	-0.72115	0.00000	8.61530
C	-1.40220	0.00000	9.83777
H	-2.49108	0.00000	9.83827
C	-0.71906	0.00000	11.05721
C	-1.40596	0.00000	-12.31290
H	-2.49361	0.00000	-12.30816
C	-0.71435	0.00000	-13.49026
H	-1.24672	0.00000	-14.43675
C	0.71435	0.00000	-13.49026
H	1.24672	0.00000	-14.43675
C	1.40596	0.00000	-12.31290
H	2.49361	0.00000	-12.30816
C	0.71906	0.00000	-11.05722
C	1.40220	0.00000	-9.83776
H	2.49108	0.00000	-9.83828
C	0.72115	0.00000	-8.61531
C	1.40473	0.00000	-7.36888
H	2.49354	0.00000	-7.37032
C	0.72620	0.00000	-6.16743
C	1.40665	0.00000	-4.90455
H	2.49551	0.00000	-4.90607
C	0.73148	0.00000	-3.70924
C	1.40533	0.00000	-2.44786
H	2.49432	0.00000	-2.44881
C	0.73493	0.00000	-1.23862
C	1.40347	0.00000	-0.00001
H	2.49253	0.00000	-0.00000
C	0.73492	0.00000	1.23864
C	1.40534	0.00000	2.44785
H	2.49432	0.00000	2.44881
C	0.73148	0.00000	3.70925
C	1.40665	0.00000	4.90455
H	2.49551	0.00000	4.90607
C	0.72619	0.00000	6.16743
C	1.40473	0.00000	7.36889
H	2.49354	0.00000	7.37032
C	0.72115	0.00000	8.61530
C	1.40220	0.00000	9.83777
H	2.49108	0.00000	9.83827
C	0.71906	0.00000	11.05721
C	-1.40596	0.00000	12.31290
H	-2.49361	0.00000	12.30815
C	-0.71436	0.00000	13.49025
H	-1.24672	0.00000	14.43675
C	0.71436	0.00000	13.49025
H	1.24672	0.00000	14.43675
C	1.40596	0.00000	12.31290
H	2.49361	0.00000	12.30815

Table S7 (cont.): Cartesian coordinates of [5]CC

C	-1.733039	1.381465	1.415659
C	-1.955452	0.158514	0.736701
C	-1.955519	0.158587	-0.736552
C	-1.733161	1.381604	-1.415409
C	-0.828098	2.233740	-0.736539
C	-0.828032	2.233665	0.736795
C	0.404004	2.399421	1.415616
C	1.493954	1.801775	0.736643
C	1.493890	1.801849	-0.736637
C	0.403878	2.399558	-1.415454
C	2.032600	0.681689	-1.415641
C	1.801595	-0.539742	-0.736765
C	1.801658	-0.539815	0.736512
C	2.032729	0.681549	1.415488
H	1.973461	0.673750	2.501146
H	0.393114	2.340572	2.501279
H	-1.680696	1.353043	-2.501073
H	-1.680475	1.352795	2.501315
H	1.973239	0.673997	-2.501295
C	0.902496	-1.398172	-1.415637
C	0.902623	-1.398315	1.415378
C	-0.330541	-1.555486	0.736576
C	-0.330607	-1.555414	-0.736741
C	-1.424586	-0.965452	1.415581
C	-1.424709	-0.965310	-1.415591
H	-1.381069	-0.924316	2.501237
H	-1.381290	-0.924067	-2.501247
H	0.392892	2.340820	-2.501122
H	0.877086	-1.344442	2.501058
H	0.876864	-1.344193	-2.501310

Table S7 (cont.): Cartesian coordinates of [6]CC

C	-1.850881	1.533752	1.401753
C	-2.357652	0.400947	0.725132
C	-2.357652	0.400947	-0.725132
C	-1.850881	1.533752	-1.401753
C	-0.830928	2.240503	-0.725168
C	-0.830928	2.240503	0.725168
C	0.403183	2.370799	1.401655
C	1.524846	1.839874	0.725168
C	1.524846	1.839874	-0.725168
C	0.403183	2.370799	-1.401655
C	2.253835	0.835695	-1.401753
C	2.357652	-0.400948	-0.725132
C	2.357652	-0.400948	0.725132
C	2.253835	0.835695	1.401753
H	2.224350	0.824771	2.489419
H	0.397933	2.339924	2.489313
H	-1.826665	1.513695	-2.489419
H	-1.826665	1.513695	2.489419
H	2.224350	0.824771	-2.489419
C	1.850881	-1.533752	-1.401753
H	1.826665	-1.513695	-2.489419
C	1.850881	-1.533752	1.401753
C	0.830928	-2.240503	-0.725168
C	0.830928	-2.240503	0.725168
C	-0.403183	-2.370799	-1.401655
C	-0.403183	-2.370799	1.401655
C	-1.524846	-1.839874	0.725168
C	-1.524846	-1.839874	-0.725168
C	-2.253835	-0.835695	1.401753
C	-2.253835	-0.835695	-1.401753
H	-0.397933	-2.339924	-2.489313
H	-0.397933	-2.339924	2.489313
H	-2.224350	-0.824771	2.489419
H	-2.224350	-0.824771	-2.489419
H	0.397933	2.339924	-2.489313
H	1.826665	-1.513695	2.489419

Table S7 (cont.): Cartesian coordinates of [7]CC

C	1.823337	-2.088902	-1.415142
C	2.768363	0.123946	-1.415208
C	1.629698	2.243627	-1.415170
C	-0.737287	2.674538	-1.415101
C	-2.548123	1.090160	-1.415197
C	-2.440736	-1.313642	-1.415244
C	-0.495539	-2.729815	-1.415105
H	1.790557	-2.051547	-2.501756
H	2.719613	0.121695	-2.501871
H	1.600861	2.204010	-2.501813
H	-0.724295	2.626856	-2.501731
H	-2.501800	1.070234	-2.501783
H	-0.486806	-2.680723	-2.501714
H	-2.396336	-1.289739	-2.501820
C	2.546579	-1.089582	-0.734129
C	2.439118	1.312857	-0.734135
C	0.495332	2.728185	-0.734179
C	-1.822232	2.087593	-0.734147
C	0.736931	-2.672971	-0.734167
C	-2.767047	-0.123926	-0.734129
C	-1.628696	-2.242200	-0.734163
C	0.736931	-2.672971	0.734167
C	-1.628696	-2.242200	0.734163
C	-2.767047	-0.123926	0.734129
C	-1.822232	2.087593	0.734147
C	0.495332	2.728185	0.734179
C	2.439118	1.312857	0.734135
C	2.546579	-1.089582	0.734129
H	-0.486806	-2.680723	2.501714
H	-2.396336	-1.289739	2.501820
H	-2.501800	1.070234	2.501783
H	-0.724295	2.626856	2.501731
H	1.600861	2.204010	2.501813
H	2.719613	0.121695	2.501871
H	1.790557	-2.051547	2.501756
C	2.768363	0.123946	1.415208
C	1.823337	-2.088902	1.415142
C	1.629698	2.243627	1.415170
C	-0.737287	2.674538	1.415101
C	-2.548123	1.090160	1.415197
C	-2.440736	-1.313642	1.415244
C	-0.495539	-2.729815	1.415105

Table S7 (cont.): Cartesian coordinates of [8]CC

C	2.797761	1.480633	1.406181
C	0.931386	3.025534	1.406063
C	-1.480677	2.797693	1.406144
C	-3.025714	0.931377	1.406054
C	-2.797814	-1.480656	1.406155
C	-0.931374	-3.025508	1.406070
C	1.480648	-2.797637	1.406176
C	3.025696	-0.931374	1.406074
H	-0.922935	-2.999082	2.493948
H	-2.773686	-1.467789	2.494023
H	-2.999292	0.922937	2.493938
H	-1.467834	2.773629	2.494013
H	0.922953	2.999144	2.493941
H	2.773439	1.467680	2.494043
H	2.999279	-0.922949	2.493960
H	1.467750	-2.773455	2.494041
C	3.142582	0.296507	0.728927
C	2.012515	2.431522	0.728913
C	-0.296504	3.142382	0.728892
C	-2.431607	2.012484	0.728898
C	-3.142619	-0.296509	0.728908
C	-2.012529	-2.431533	0.728907
C	0.296500	-3.142334	0.728909
C	2.431580	-2.012464	0.728916
C	2.012529	2.431533	-0.728907
C	3.142619	0.296509	-0.728908
C	-0.296500	3.142334	-0.728909
C	2.431607	-2.012484	-0.728898
C	0.296504	-3.142382	-0.728892
C	-2.012515	-2.431522	-0.728913
C	-3.142582	-0.296507	-0.728927
C	-2.431580	2.012464	-0.728916
H	-0.922953	-2.999144	-2.493941
H	-2.773439	-1.467680	-2.494043
H	-2.999279	0.922949	-2.493960
H	-1.467750	2.773454	-2.494041
H	0.922935	2.999082	-2.493948
H	2.773685	1.467789	-2.494023
H	2.999292	-0.922937	-2.493938
H	1.467834	-2.773629	-2.494013
C	2.797814	1.480656	-1.406155
C	0.931374	3.025508	-1.406070
C	-1.480648	2.797637	-1.406176
C	-3.025696	0.931374	-1.406074
C	-2.797761	-1.480633	-1.406181
C	3.025714	-0.931377	-1.406054
C	-0.931386	-3.025534	-1.406063
C	1.480677	-2.797693	-1.406144

Table S7 (cont.): Cartesian coordinates of [9]CC

C	3.067253	1.414196	-1.772268
C	3.487031	1.414083	0.615257
C	2.277287	1.414205	2.715830
C	0.000000	1.414282	3.547034
C	-2.277287	1.414205	2.715830
C	-3.487031	1.414083	0.615257
C	-3.067253	1.414196	-1.772268
C	-1.212023	1.414122	-3.332633
C	1.212023	1.414122	-3.332633
H	-3.032046	2.501500	-1.752032
H	-3.447586	2.501432	0.608311
H	-2.251630	2.501546	2.685018
H	0.000000	2.501563	3.506023
H	2.251630	2.501546	2.685018
H	3.447586	2.501432	0.608311
H	3.032046	2.501500	-1.752032
H	1.198154	2.501459	-3.295013
H	-1.198154	2.501459	-3.295013
C	0.000000	0.733013	-3.545688
C	2.276946	0.733020	-2.715317
C	3.486464	0.733063	-0.615194
C	1.211648	0.733124	3.332161
C	3.065927	0.732966	1.771608
C	-1.211648	0.733124	3.332161
C	-3.065927	0.732966	1.771608
C	-3.486464	0.733063	-0.615194
C	-2.276946	0.733020	-2.715317
C	0.000000	-0.733013	-3.545688
C	2.276946	-0.733020	-2.715317
C	3.486464	-0.733063	-0.615194
C	3.065927	-0.732966	1.771608
C	1.211648	-0.733124	3.332161
C	-1.211648	-0.733124	3.332161
C	-3.065927	-0.732966	1.771608
C	-3.486464	-0.733063	-0.615194
C	-2.276946	-0.733020	-2.715317
H	-3.032046	-2.501500	-1.752032
H	-3.447586	-2.501432	0.608311
H	-2.251630	-2.501546	2.685018
H	1.198154	-2.501459	-3.295013
H	3.032046	-2.501500	-1.752032
H	3.447586	-2.501432	0.608311
H	2.251630	-2.501546	2.685018
H	0.000000	-2.501563	3.506023
H	-1.198154	-2.501459	-3.295013
C	1.212023	-1.414122	-3.332633
C	3.067253	-1.414196	-1.772268
C	3.487031	-1.414083	0.615257
C	2.277287	-1.414205	2.715830
C	-2.277287	-1.414205	2.715830
C	-3.487031	-1.414083	0.615257
C	-3.067253	-1.414196	-1.772268
C	-1.212023	-1.414122	-3.332633
C	0.000000	-1.414282	3.547034

Table S7 (cont.): Cartesian coordinates of [10]CC

C	-3.247010	2.224237	1.407993
C	-1.319232	3.707037	1.407846
C	1.111934	3.774539	1.408084
C	3.118587	2.400180	1.408089
C	3.934122	0.109024	1.408289
C	3.246908	-2.224070	1.408427
C	1.319130	-3.706865	1.408325
C	-1.112033	-3.774368	1.408428
C	-3.118691	-2.400015	1.408163
C	-3.934227	-0.108859	1.408065
H	3.098052	2.384299	2.496081
H	3.908051	0.108427	2.496273
H	3.225557	-2.209518	2.496413
H	-1.310575	3.682850	2.495844
H	-3.225763	2.209828	2.495983
H	-3.908262	-0.108155	2.496052
H	-3.098222	-2.384035	2.496155
H	-1.104902	-3.749655	2.496418
H	1.310404	-3.682523	2.496319
H	1.104757	3.749958	2.496077
C	-2.397160	3.113338	0.730549
C	-0.109050	3.927278	0.730504
C	2.220975	3.241939	0.730649
C	3.702410	1.317564	0.730747
C	3.770305	-1.110114	0.730915
C	2.397141	-3.113274	0.731017
C	0.109033	-3.927211	0.730928
C	-2.220994	-3.241880	0.730869
C	-3.702432	-1.317505	0.730674
C	-3.770327	1.110174	0.730581
C	-2.397106	3.113297	-0.731044
C	-0.108971	3.927217	-0.730963
C	3.702489	1.317453	-0.730680
C	3.770354	-1.110234	-0.730576
C	2.397173	-3.113391	-0.730554
C	0.109041	-3.927310	-0.730524
C	-2.220990	-3.241947	-0.730672
C	-3.702423	-1.317555	-0.730766
C	-3.770286	1.110133	-0.730932
C	2.221059	3.241847	-0.730893
H	3.226177	-2.209381	-2.495973
H	3.908307	0.108743	-2.496037
H	3.097952	2.384571	-2.496155
H	1.104369	3.749957	-2.496422
H	-1.311053	3.682502	-2.496322
H	-3.226088	2.209153	-2.496406
H	-3.908217	-0.109013	-2.496260
H	-3.097826	-2.384854	-2.496081
H	-1.104220	-3.750203	-2.496081
H	1.311177	-3.682714	-2.495844
C	-1.319770	3.706729	-1.408314
C	-3.247346	2.223606	-1.408405
C	-3.934185	-0.109635	-1.408262
C	-3.118276	-2.400696	-1.408075
C	-1.111367	-3.774754	-1.408075
C	1.319835	-3.706866	-1.407834
C	3.247412	-2.223745	-1.407971
C	3.934249	0.109494	-1.408039
C	3.118340	2.400554	-1.408149
C	1.111432	3.774614	-1.408419

Table S7 (cont.): Cartesian coordinates of [11]CC

C	-3.631286	2.335405	1.413355
C	-4.315835	0.000000	1.413442
C	-3.631286	-2.335405	1.413355
C	-1.793910	-3.931435	1.413377
C	0.614724	-4.278520	1.413402
C	2.827610	-3.265337	1.413529
C	4.141036	-1.216846	1.413345
C	4.141036	1.216844	1.413345
C	2.827611	3.265337	1.413529
C	0.614726	4.278519	1.413402
C	-1.793908	3.931435	1.413377
H	-1.779290	3.899877	-2.500886
H	-1.779290	3.899877	2.500886
H	0.609580	4.243465	-2.500901
H	0.609580	4.243465	2.500901
H	2.804633	3.238855	-2.501026
H	2.804633	3.238855	2.501026
H	4.108040	1.207244	-2.500869
H	4.108040	1.207244	2.500869
H	4.108041	-1.207244	-2.500869
H	4.108041	-1.207244	2.500869
H	2.804633	-3.238855	-2.501026
C	-4.140676	1.216660	0.732477
C	-4.140676	-1.216658	0.732477
C	-2.827314	-3.265083	0.732365
C	-0.614503	-4.278009	0.732454
C	1.793970	-3.931527	0.732503
C	3.630520	-2.335019	0.732391
C	4.315328	0.000000	0.732495
C	3.630519	2.335018	0.732391
C	1.793971	3.931528	0.732503
C	-0.614501	4.278009	0.732454
C	-2.827313	3.265083	0.732365
C	-4.140676	1.216660	-0.732477
C	-4.140676	-1.216658	-0.732477
C	-2.827314	-3.265083	-0.732365
C	-0.614503	-4.278009	-0.732454
C	1.793970	-3.931527	-0.732503
C	3.630520	-2.335019	-0.732391
C	4.315328	0.000000	-0.732495
C	3.630519	2.335018	-0.732391
C	1.793971	3.931528	-0.732503
C	-0.614501	4.278009	-0.732454
C	-2.827313	3.265083	-0.732365
H	2.804633	-3.238855	2.501026
H	0.609580	-4.243465	-2.500901
H	0.609580	-4.243465	2.500901
H	-1.779291	-3.899876	-2.500886
H	-1.779291	-3.899876	2.500886
H	-3.601726	-2.316645	-2.500862
H	-3.601726	-2.316645	2.500862
H	-4.281536	0.000001	2.500962
H	-4.281536	0.000001	-2.500962
H	-3.601725	2.316646	-2.500862
H	-3.601725	2.316646	2.500862
C	-3.631286	-2.335405	-1.413355
C	-1.793910	-3.931435	-1.413377
C	0.614724	-4.278520	-1.413402
C	2.827610	-3.265337	-1.413529
C	4.141036	-1.216846	-1.413345
C	4.141036	1.216844	-1.413345
C	2.827611	3.265337	-1.413529
C	0.614726	4.278519	-1.413402
C	-1.793908	3.931435	-1.413377
C	-3.631286	2.335405	-1.413355
C	-4.315835	0.000000	-1.413442

Table S7 (cont.): Cartesian coordinates of cyclo[a]decacene

C	-2.421996	-2.445534	1.236129
C	-0.202755	-3.351283	1.694465
C	2.173125	-2.814102	1.800180
C	3.756673	-0.977951	1.576297
C	2.395767	3.365109	0.954652
C	0.057923	4.046136	1.017974
C	-2.211625	3.256225	1.440976
C	-3.837023	0.076056	1.872607
H	-4.103880	-0.608465	2.673451
C	-3.184863	-1.793489	0.268947
C	-1.335106	-3.267885	0.853103
C	1.076419	-3.423710	1.131693
C	3.143031	-2.144089	1.050668
C	3.230885	2.395751	0.382557
C	1.210921	3.745110	0.277077
C	-1.204078	3.658189	0.528704
C	-3.647155	1.393645	2.131794
C	-3.672807	-0.446829	0.535513
C	-3.088111	-2.237985	-1.100522
C	-1.204282	-3.658144	-0.528699
C	1.210713	-3.745175	-0.277071
C	3.230743	-2.395908	-0.382556
C	3.845090	1.425980	1.207225
C	3.143158	2.143937	-1.050665
C	1.076612	3.423658	-1.131690
C	-1.334923	3.267946	-0.853101
C	-3.087991	2.238142	1.100518
C	-3.672772	0.447020	-0.535522
C	0.057701	-4.046159	-1.017965
C	2.395575	-3.365226	-0.954649
C	3.844998	-1.426172	-1.207223
C	3.990455	0.111041	0.721485
C	3.756731	0.977762	-1.576296
C	2.173291	2.814002	-1.800178
C	-0.202566	3.351291	-1.694463
C	-2.421856	2.445654	-1.236130
C	-3.184757	1.793650	-0.268951
C	-2.211804	-3.256124	-1.440975
H	-2.439021	2.086789	-2.261578
H	-2.108206	3.533936	2.488226
H	-2.108399	-3.533847	-2.488223
H	-0.300725	3.043187	-2.733358
H	0.159011	4.270316	2.077898
H	2.462896	3.550921	2.024414
H	2.072077	2.580526	-2.857832
H	2.462689	-3.551040	-2.024411
H	2.071924	-2.580617	2.857834
H	0.158777	-4.270352	-2.077887
H	-0.300901	-3.043169	2.733357
H	-3.753262	1.786545	3.139668
H	-2.439145	-2.086668	2.261576
C	-3.647212	-1.393453	-2.131803
C	-3.836995	-0.075853	-1.872618
H	-3.753318	-1.786340	-3.139681
H	-4.103778	0.608687	-2.673472
C	3.990447	-0.111242	-0.721484
H	3.704330	0.800276	-2.648149
H	3.858531	-1.591163	-2.282278
H	3.704285	-0.800460	2.648151
H	3.858639	1.590976	2.282278

Table S7 (cont.): Cartesian coordinates of cyclo[a]undecacene

C	2.914647	-2.549017	-1.136010
C	0.799417	-3.687932	-1.586704
C	-1.630882	-3.540176	-1.772417
C	-3.596866	-2.100233	-1.678130
C	-4.402068	0.183093	-1.398783
C	-3.738285	2.510127	-1.109249
C	-1.856055	4.055576	-0.988781
C	0.565809	4.319120	-1.143696
C	2.731715	3.266630	-1.570288
C	4.233648	-0.004886	-1.876518
H	4.490052	-0.726563	-2.647379
C	3.626299	-1.817989	-0.193056
C	1.893290	-3.446734	-0.732136
C	-0.471392	-3.930749	-1.051201
C	-2.752562	-3.077798	-1.085602
C	-4.177998	-1.112656	-0.877570
C	-4.217953	1.304529	-0.569653
C	-2.854783	3.312961	-0.348995
C	-0.596601	4.227400	-0.363213
C	1.779071	3.796088	-0.662478
C	4.063064	1.301467	-2.192577
C	4.076826	-0.467152	-0.514501
C	3.541211	-2.208937	1.194796
C	1.779108	-3.796073	0.662479
C	-0.596560	-4.227404	0.363215
C	-2.854750	-3.312983	0.348996
C	-4.217940	-1.304565	0.569652
C	-4.178010	1.112621	0.877568
C	-2.752592	3.077775	1.085602
C	-0.471430	3.930745	1.051203
C	1.893256	3.446748	0.732137
C	3.541189	2.208969	-1.194796
C	4.076823	0.467189	0.514501
C	0.565850	-4.319116	1.143697
C	-1.856016	-4.055591	0.988783
C	-3.738262	-2.510160	1.109248
C	-4.402068	-0.183132	1.398781
C	-3.596888	2.100202	1.678129
C	-1.630916	3.540162	1.772417
C	0.799381	3.687935	1.586705
C	2.914622	2.549040	1.136009
C	3.626281	1.818021	0.193056
C	2.731747	-3.266607	1.570288
H	2.919695	2.234649	2.176068
H	2.638374	3.511795	-2.626572
H	2.638410	-3.511772	2.626572
H	0.881199	3.404875	2.634196
H	0.469234	4.520682	-2.208614
H	-1.930167	4.223647	-2.061083
H	-1.532681	3.316619	2.832617
H	-3.525636	1.933582	2.750759
H	-3.773902	2.653539	-2.186960
H	-4.384752	-0.321720	2.477550
H	-4.384754	0.321682	-2.477551
H	-3.525616	-1.933614	-2.750761
H	-3.773878	-2.653571	2.186959
H	-1.930127	-4.223661	2.061085
H	-1.532648	-3.316634	-2.832617
H	0.469276	-4.520677	2.208616
H	0.881233	-3.404873	-2.634196
H	4.171144	1.648234	-3.217053
H	2.919718	-2.234628	-2.176069
C	4.063077	-1.301431	2.192576
C	4.233648	0.004925	1.876517
H	4.171161	-1.648196	3.217052
H	4.490044	0.726604	2.647379

Table S7 (cont.): Cartesian coordinates of [3]cyclobenzo[a]anthracene

C	3.22273	-2.60512	1.18875
C	2.75624	-3.11851	-0.05436
C	1.49975	-3.88153	-0.05451
C	0.82898	-4.05936	1.18850
C	2.72635	-3.18522	2.42246
C	1.57246	-3.88645	2.42234
H	3.23786	-2.94861	3.35207
C	0.75356	-4.09304	-1.21883
C	-0.56776	-4.12324	1.21845
C	-1.32277	-3.94568	0.05421
C	-0.64463	-4.09259	-1.18885
H	1.23250	-4.05300	-2.19326
H	-1.04810	-4.10456	2.19282
H	1.12661	-4.23145	3.35185
C	-2.61238	-3.23991	0.05417
C	-1.39519	-3.95341	-2.42266
C	-2.57974	-3.30530	-2.42268
C	-3.10166	-2.74805	-1.18893
H	-0.93438	-4.27817	-3.35218
H	-3.10160	-3.09217	-3.35224
C	3.28796	-2.55347	-1.21851
C	3.92232	-1.39450	1.21887
C	3.93098	-1.31190	-1.18837
C	4.11209	-0.64225	0.05477
H	3.03129	-2.95974	-2.19299
H	4.12678	-0.95962	2.19333
C	4.15242	-0.58136	-2.42214
C	4.07872	0.82738	0.05480
C	3.86735	1.48816	-1.18827
C	4.12184	0.76854	-2.42209
H	4.17211	1.32996	-3.35168
H	4.22830	-1.13985	-3.35173
C	3.85513	1.57024	1.21903
C	3.16893	2.69941	-1.21835
C	2.61238	3.23991	-0.05417
C	3.10166	2.74805	1.18893
H	2.89460	3.09394	-2.19284
H	4.07915	1.14509	2.19350
C	1.32277	3.94568	-0.05421
C	2.57974	3.30530	2.42268
C	1.39519	3.95341	2.42266
C	0.64463	4.09259	1.18885
H	3.10161	3.09217	3.35224
H	0.93439	4.27818	3.35218
C	-3.16893	-2.69941	1.21835
C	-3.85513	-1.57024	-1.21903
C	-3.86735	-1.48816	1.18827
C	-4.07872	-0.82738	-0.05481
H	-4.07915	-1.14509	-2.19350
H	-2.89460	-3.09394	2.19284
C	-4.12184	-0.76854	2.42209
C	-4.11209	0.64225	-0.05478
C	-4.15243	0.58136	2.42214
C	-3.93098	1.31190	1.18837
H	-4.17212	-1.32996	3.35168
H	-4.22830	1.13985	3.35173
C	-0.75356	4.09304	1.21883
C	0.56776	4.12325	-1.21845
C	-0.82898	4.05936	-1.18850
C	-1.49975	3.88154	0.05450
H	1.04810	4.10456	-2.19282
H	-1.23250	4.05300	2.19326
C	-1.57246	3.88645	-2.42234
C	-2.75624	3.11851	0.05436
C	-3.22273	2.60512	-1.18875
C	-2.72635	3.18521	-2.42246
H	-1.12661	4.23144	-3.35185
H	-3.23786	2.94860	-3.35207
C	-3.92232	1.39450	-1.21887
H	-4.12678	0.95962	-2.19333
C	-3.28796	2.55346	1.21851
H	-3.03129	2.95974	2.19299

Table S7 (cont.): Cartesian coordinates of [3]cyclochrysene

C	-3.347889	-1.935089	-1.786665
C	-2.543610	-2.842072	-2.406058
C	-1.443896	-3.402523	-1.692969
C	-0.276523	-3.804225	-2.405706
C	0.934377	-3.752438	-1.785995
C	3.350425	-1.931851	-1.786285
C	3.734101	-0.782148	-2.405987
C	3.669699	0.450729	-1.693210
C	3.433497	1.662341	-2.406166
C	2.782839	2.685042	-1.786618
C	-0.002338	3.866970	-1.786345
C	-1.190011	3.624355	-2.405720
C	-2.225303	2.951993	-1.692830
C	-3.157098	2.142169	-2.405706
C	-3.717790	1.067487	-1.786297
C	-1.029877	3.482985	0.382163
C	-0.934055	3.751743	1.786468
C	0.156034	3.628814	-0.382121
C	-2.196049	2.913249	-0.288152
C	0.276961	3.803692	2.405954
C	1.425440	3.358110	0.288210
C	-3.065410	1.949516	0.382151
C	1.444288	3.402412	1.692921
C	-3.350479	1.931519	1.786419
C	2.502234	2.633604	-0.382292
C	-3.532529	0.849769	-0.382099
C	2.544376	2.842295	2.405718
C	-3.734375	0.781752	2.405877
C	3.221747	1.679611	0.381871
C	3.348681	1.935475	1.786137
C	3.621971	0.444995	-0.288496
C	3.532599	-0.849724	0.382041
C	-3.621946	-0.445056	0.288208
C	-3.669990	-0.451015	1.692911
C	3.065472	-1.949629	-0.381987
C	-3.221520	-1.679538	-0.382298
C	-3.434280	-1.662837	2.405695
C	-2.502362	-2.633725	0.381952
C	-2.783620	-2.685527	1.786137
C	-1.425347	-3.358153	-0.288255
C	-0.156054	-3.628684	0.382384
C	0.002082	-3.866198	1.786739
C	1.029990	-3.483184	-0.381765
C	1.189716	-3.623529	2.406171
C	2.196092	-2.913238	0.288487
C	3.717757	-1.067130	1.786304
C	2.225201	-2.951594	1.693177
C	3.156966	-2.141630	2.405929
H	0.814090	4.274816	-2.363222
H	-1.304705	3.800389	-3.472102
H	-2.638203	-3.028889	-3.472570
H	-0.344979	-4.002459	-3.472158
H	1.825289	-3.950598	-2.362752
H	3.295063	-2.842823	-2.363086
H	3.943464	-0.770970	-3.472446
H	3.639128	1.702037	-3.472667
H	2.508266	3.555259	-2.363628
H	-3.294577	2.300810	-3.472126
H	-4.334753	0.394969	-2.363164
H	-1.824888	3.949394	2.363514
H	0.345560	4.001657	3.472446
H	2.639313	3.029300	3.472166
H	4.110180	1.432437	2.362974
H	-3.640404	-1.702765	3.472092
H	-2.509644	-3.556098	2.362920
H	-0.814508	-4.273448	2.363784
H	1.304195	-3.799078	3.472657
H	3.294305	-2.299975	3.472411
H	-3.295131	2.842411	2.363358
H	-3.943927	0.770426	3.472297
H	-4.108894	-1.431670	-2.363807
H	4.334605	-0.394464	2.363107

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