Structural Index of (Anti)aromaticity for Fused Polycyclic Hydrocarbons in the Triplet and Singlet States: HOMA or HOMER?

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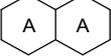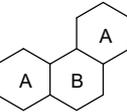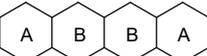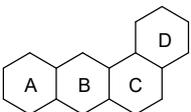
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Supplementary Information

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Table S1. Symmetry point group (PG), HOMA, HOMER, Shannon aromaticity index (SA), electron density of delocalized bond per atom (EDDB$_P$, in e), multicenter index (MCI) and NICS(1)$_{zz}$ (in ppm) calculated for S$_0$ state of given polycycles at the CAM-B3LYP/6-311+G(d,p) level of theory. ″Peri″ means molecular perimeter.

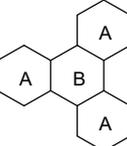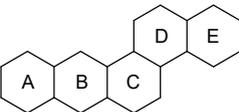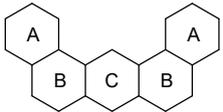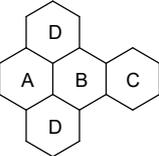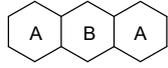| Compound	PG	HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$
	D$_{2h}$	A: 0.819 peri:0.835	-0.858 -1.265	0.0008 0.0009	0.5039 0.5302	0.071	-29.1 /
	D$_{2h}$	A: 0.646 B: 0.829 peri: 0.767	-1.022 -0.256 -1.265	0.0017 0.0005 0.0013	0.3411 0.5404 0.4310	0.050 0.053	-25.3 -35.3 /
	C$_{2v}$	A: 0.910 B: 0.503 peri: 0.754	-0.862 -0.502 -1.077	0.0004 0.0018 0.0012	0.6574 0.2354 0.5224	0.086 0.029	-29.1 -19.9 /
	D$_{2h}$	A: 0.529 B: 0.745 peri: 0.746	-1.177 -0.269 -1.295	0.0022 0.0008 0.0014	0.2774 0.4443 0.4154	0.041 0.044	-22.0 -35.0 /
	C$_s$	A: 0.735 B: 0.850 C: 0.317 D: 0.939 peri: 0.719	-0.940 -0.352 -0.627 -0.866 -1.166	0.0013 0.0004 0.0024 0.0003 0.0014	0.4020 0.5326 0.1945 0.7125 0.4651	0.058 0.056 0.021 0.093	-26.7 -32.4 -13.8 -28.3 /
	C$_{2h}$	A: 0.885 B: 0.623 peri: 0.715	-0.863 -0.463 -0.971	0.0005 0.0014 0.0014	0.6065 0.3206 0.4916	0.082 0.039	-28.6 -22.1 /
	C$_{2v}$^{a}	A: 0.837 B: 0.421 peri: 0.607	-0.858 -0.741 -1.305	0.0008 0.0025 0.0021	0.6243 0.3181 0.5048	0.082 0.040	-29.3 -22.4 /
	D$_{2h}$	A: 0.921 B: 0.592 peri: 0.761	-0.483 -0.364 -1.213	0.0002 0.0014 0.0012	0.6684 0.2861 0.4863	0.071 0.029	-35.7 -15.8 /
	D$_{3h}$	A: 0.940 B: 0.162 peri: 0.694	-0.950 0.186 -0.948	0.0003 0.0014 0.0014	0.7221 0.1366 0.5702	0.096 0.013	-26.4 -9.4 /
	D$_{2h}$^{b}	A: 0.454 B: 0.663 C: 0.727 peri: 0.747	-1.284 -0.365 -0.156 -1.285	0.0026 0.0011 0.0007 0.0014	0.2476 0.3608 0.4158 0.4199	0.036 0.036 0.037	-19.3 -32.9 -37.7 /
	C$_s$	A: 0.709 B: 0.856 C: 0.436 D: 0.669 E: 0.870 peri: 0.695	-0.969 -0.308 -0.614 -0.460 -0.862 -1.050	0.0014 0.0004 0.0021 0.0013 0.0006 0.0015	0.3789 0.5379 0.2290 0.3496 0.5841 0.4415	0.055 0.056 0.027 0.044 0.079	-26.1 -32.9 -16.3 -22.6 -28.3 /
	C$_{2v}$	A: 0.928 B: 0.404 C: 0.903 peri: 0.687	-0.858 -0.567 -0.394 -1.096	0.0003 0.0022 0.0003 0.0015	0.6943 0.2128 0.6153 0.4743	0.091 0.024 0.065	-28.2 -15.9 -31.0 /
	C$_{2v}$	A: 0.564 B: 0.287 C: 0.939 D: 0.922 peri: 0.713	-0.418 0.432 -0.949 -0.599 -1.109	0.0016 0.0010 0.0003 0.0003 0.0014	0.2708 0.2013 0.7164 0.6861 0.5288	0.029 0.013 0.094 0.076	-16.3 -5.7 -25.4 -32.4
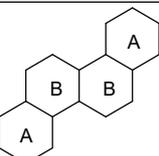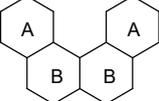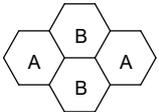
Compound	PG	SD	HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$
(rings: C C / A B A / C C)	D$_{2h}$[c]	A: 0.793	-0.289	0.0007	0.4203	0.045	-30.5	
		B: 0.679	0.822	0.0000	0.3707	0.018	-5.4	
		C: 0.793	-0.829	0.0007	0.4204	0.045	-30.5	
		peri: 0.759	-0.973	0.0011	0.4171		/	

[a] i 155.6 cm^{-1} (HH steric interaction). [b] RHF → UHF. [c] i 111.0 cm^{-1} (out-of-plane central ring).

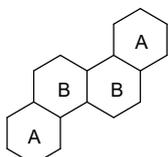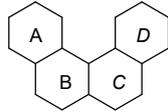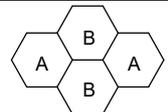**Table S2.** Symmetry point group (PG), spin density at carbon atoms (SD), HOMA, HOMER, Shannon aromaticity index (SA), electron density of delocalized bond per atom (EDDB$_P$, in e), multicenter index (MCI) and NICS(1)$_{zz}$ (in ppm) calculated for T$_1$ state of given polycycles at the UCAM-B3LYP/6-311+G(d,p) (nor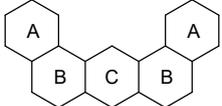mal font) and M06-2X/6-311+G(d,p) (*italic*) levels of theory. ″Peri″ means molecular perimeter. NICS is calculated only with UCAM-B3LYP.

Compound	PG	SD	HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$
(rings: A A)	D$_{2h}$	A: 0.91	0.540	-0.615	0.0018	0.2397	0.031	26.1
		0.93	*0.525*	*-0.469*	*0.0017*	*0.2509*	*0.031*	
		peri: 1.88	0.638	-0.911	0.0018	0.3467		/
		1.89	*0.623*	*-0.735*	*0.0017*	*0.3552*		
(rings: A B A)	D$_{2h}$	A: 0.50	0.877	-0.716	0.0005	0.5560	0.069	-5.1
		0.51	*0.874*	*-0.518*	*0.0005*	*0.5762*	*0.071*	
		B: 0.95	0.530	0.962	0.0000	0.3565	0.011	25.9
		1.00	*0.481*	*0.984*	*0.0000*	*0.3567*	*0.011*	
		peri: 1.89	0.835	-0.480	0.0007	0.5572		/
		1.90	*0.816*	*-0.303*	*0.0006*	*0.5692*		
(rings: A B / A)	C$_{2v}$	A: 0.51	0.774	-0.692	0.0009	0.5168	0.054	8.5
		0.52	*0.760*	*-0.525*	*0.0009*	*0.5213*	*0.055*	
		B: 1.14	-0.101	-0.818	0.0031	0.1325	0.007	36.6
		1.11	*-0.104*	*-0.704*	*0.0029*	*0.1395*	*0.007*	
		peri: 1.90	0.560	-1.219	0.0021	0.4404		/
		1.88	*0.558*	*-1.021*	*0.0020*	*0.4456*		
(rings: A B B A)	D$_{2h}$	A: 0.34	0.948	-0.679	0.0001	0.7165	0.082	-17.7
		0.35	*0.932*	*-0.458*	*0.0002*	*0.7081*	*0.080*	
		B: 0.65	0.544	0.267	0.0008	0.2650	0.018	8.9
		0.67	*0.525*	*0.341*	*0.0008*	*0.2829*	*0.019*	
		peri: 1.90	0.879	-0.492	0.0004	0.6289		/
		1.90	*0.871*	*-0.310*	*0.0004*	*0.6407*		
(rings: A B C / D)	C$_s$	A: 0.57	0.829	-0.721	0.0007	0.4602	0.061	4.8
		0.55	*0.846*	*-0.529*	*0.0006*	*0.5109*	*0.065*	
		B: 1.00	0.544	0.770	0.0003	0.3146	0.012	35.1
		1.05	*0.501*	*0.847*	*0.0002*	*0.3262*	*0.011*	
		C: 0.39	0.820	-0.114	0.0005	0.5606	0.050	-14.3
		0.39	*0.798*	*0.035*	*0.0004*	*0.5595*	*0.050*	
		D: 0.17	0.744	-0.890	0.0012	0.4408	0.061	-21.5
		0.19	*0.717*	*-0.707*	*0.0012*	*0.4331*	*0.060*	
		peri: 1.90	0.769	-0.554	0.0010	0.4936		/
		1.91	*0.753*	*-0.376*	*0.0009*	*0.5056*		
(rings: A / B B / A)	C$_{2h}$[a]	A: 0.29	0.944	-0.770	0.0002	0.7077	0.086	-7.0
		0.29	*0.935*	*-0.557*	*0.0002*	*0.7099*	*0.086*	
		B: 0.93	0.014	-0.847	0.0030	0.2279	0.009	32.4
		0.91	*0.007*	*-0.717*	*0.0028*	*0.2347*	*0.010*	
		peri: 1.91	0.632	-1.106	0.0017	0.4908		/
		1.92	*0.624*	*-0.898*	*0.0017*	*0.5221*		
(rings: A D / B C)	C$_{2v}$/C_s[b]	A: 0.38	0.838	-0.800	0.0008	0.6023	0.076	3.4
		0.47	*0.781*	*-0.602*	*0.0009*	*0.5168*	*0.068*	
		B: 0.95	-0.343	-1.520	0.0043	0.2224	0.008	40.0
		1.06	*-0.245*	*-1.163*	*0.0038*	*0.2559*	*0.011*	
		C: 0.70	*-0.248*	*-1.307*	*0.0041*	*0.1719*	*0.010*	
		D: 0.32	*0.823*	*-0.531*	*0.0007*	*0.6553*	*0.075*	
		peri: 1.92	0.678	-1.087	0.0017	0.5248		/
		1.92	*0.590*	*-1.080*	*0.0021*	*0.4655*		
(rings: B / A A / B)	D$_{2h}$	A: 0.68	0.586	0.021	0.0010	0.3634	0.022	25.7
		0.69	*0.562*	*0.096*	*0.0010*	*0.3712*	*0.022*	
		B: 0.33	0.836	-0.230	0.0005	0.5019	0.050	-5.4

Structure	Symmetry	Ring						
		0.34	0.821	-0.048	0.0004	0.5116	0.050	
		peri: 1.90	0.738	-0.734	0.0011	0.4305		/
		1.90	*0.725*	*-0.547*	*0.0011*	*0.4418*		
rings A B, C (top), C (bottom)	C_{2v}/C_s [c]	A: 0.16	0.866	-0.403	0.0005	0.7610	0.013	-0.2
		0.11	*0.971*	*-0.703*	*0.0001*	*0.7895*	*0.037*	
		B: 0.81	0.463	0.727	0.0004	0.1349	0.040	53.6
		0.72	*-0.296*	*-0.699*	*0.0028*	*0.1097*	*0.039*	
		C: 0.88	0.808	-0.371	0.0006	0.3449	0.032	53.4
		0.90	*0.308*	*-1.145*	*0.0028*	*0.3004*	*0.020*	
		peri: 1.92	0.779	-0.350	0.0007	0.4285		/
		1.92	*0.531*	*-1.198*	*0.0022*	*0.3984*		
rings A B C B A	D_{2h}	A: 0.23	0.912	-0.707	0.0003	0.6479	0.078	-23.1
		0.24	*0.894*	*-0.494*	*0.0004*	*0.6392*	*0.076*	
		B: 0.44	0.640	-0.204	0.0011	0.2950	0.028	-7.1
		0.45	*0.625*	*-0.067*	*0.0010*	*0.3134*	*0.029*	
		C: 0.63	0.481	0.603	0.0005	0.2823	0.011	9.8
		0.68	*0.454*	*0.623*	*0.0005*	*0.2896*	*0.012*	
		peri: 1.90	0.872	-0.584	0.0005	0.5804		/
		1.91	*0.866*	*-0.400*	*0.0005*	*0.5931*		
rings A B C, D E	C_s	A: 0.52	0.869	-0.709	0.0005	0.5258	0.066	0.3
		0.51	*0.837*	*-0.510*	*0.0005*	*0.5564*	*0.069*	
		B: 0.95	0.568	0.894	0.0001	0.3486	0.012	32.3
		0.98	*0.527*	*0.936*	*0.0001*	*0.3558*	*0.012*	
		C: 0.43	0.826	-0.175	0.0005	0.5760	0.052	-8.4
		0.44	*0.799*	*-0.14*	*0.0005*	*0.5720*	*0.052*	
		D: 0.23	0.395	-0.474	0.0021	0.2318	0.024	-11.4
		0.23	*0.359*	*-0.369*	*0.0021*	*0.2382*	*0.024*	
		E: 0.04	0.933	-0.862	0.0003	0.6951	0.090	-27.2
		0.05	*0.923*	*-0.642*	*0.0003*	*0.6956*	*0.090*	
		peri: 1.90	0.743	-0.634	0.0011	0.5085		/
		1.91	*0.728*	*-0.456*	*0.0011*	*0.5183*		
rings A (top), B C B, A (top)	C_{2v}	A: 0.21	0.691	-0.945	0.0015	0.3927	0.054	-17.3
		0.21	*0.677*	*-0.752*	*0.0014*	*0.3986*	*0.055*	
		B: 0.41	0.830	-0.131	0.0004	0.5617	0.050	-7.6
		0.41	*0.804*	*0.007*	*0.0004*	*0.5603*	*0.049*	
		C: 1.13	0.527	0.729	0.0004	0.2903	0.010	53.0
		1.15	*0.485*	*0.759*	*0.0004*	*0.2970*	*0.011*	
		peri: 1.91	0.731	-0.604	0.0012	0.4713		/
		1.91	*0.713*	*-0.436*	*0.0011*	*0.4774*		
rings D (top), A B C, D (bottom)	C_{2v}	A: 0.56	0.550	-0.338	0.0015	0.2729	0.027	12.7
		0.52	*0.571*	*-0.162*	*0.0013*	*0.3128*	*0.030*	
		B: 0.22	0.695	0.521	0.0003	0.4054	0.033	-17.0
		0.24	*0.658*	*0.638*	*0.0003*	*0.4211*	*0.033*	
		C: 0.12	0.780	-0.910	0.0011	0.4828	0.065	-26.3
		0.15	*0.755*	*-0.711*	*0.0011*	*0.4731*	*0.064*	
		D: 0.65	0.613	-0.233	0.0012	0.3681	0.027	26.7
		0.67	*0.589*	*-0.107*	*0.0012*	*0.3755*	*0.028*	
		peri: 1.90	0.700	-0.745	0.0013	0.4155		/
		1.90	*0.690*	*-0.574*	*0.0013*	*0.4255*		
rings C C (top), A B A, C C (bottom)	D_{2h} [d]	A: 0.49	0.260	-0.763	0.0027	0.1782	0.013	57.6
		0.39	*0.723*	*-0.107*	*0.0008*	*0.3709*	*0.037*	
		B: 0.13	0.857	0.289	0.0001	0.5126	0.040	3.3
		0.15	*0.823*	*0.411*	*0.0001*	*0.4894*	*0.039*	
		C: 0.42	0.734	-0.022	0.0006	0.4179	0.032	44.7
		0.47	*0.488*	*-0.121*	*0.0014*	*0.2688*	*0.020*	
		peri: 1.80	0.658	-1.246	0.0018	0.4099		/
		1.79	*0.662*	*-0.974*	*0.0016*	*0.3303*		

[a] i 45.0/*53.3* cm⁻¹ (out-of-plane due to HH steric interactions). [b] i 179.2/*210.3* cm⁻¹ (HH steric interaction). [c] Non-planar. [d] i 294.6/*588.9* cm⁻¹ (out-of-plane central ring), i 170.7/*363.5* cm⁻¹ (bond lengths).

Table S3. Symmetry point group (PG), HOMA, HOMER, Shannon aromaticity index (SA), electron density of delocalized bond per atom (EDDB$_P$, in e), multicenter index (MCI) and NICS(1)$_{zz}$ (in ppm) calculated for S$_0$ state of given polycycles at the CAM-B3LYP/6-311+G(d,p) level of theory. ″Peri″ means molecular perimeter.

Compound	PG	HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$
(A–B)	C$_{2v}$	A: 0.679	-2.073	0.0016	0.3878	0.090	-8.1
		B: -1.499	-4.639	0.0116	0.0221	0.015	46.5
		peri: -0.430	-4.043	0.0080	0.2145		/
(A–B–A)	D$_{2h}$	A: 0.858	-1.425	0.0006	0.6399	0.104	-14.1
		B: -0.954	-1.630	0.0063	0.0353	0.016	36.6
		peri: 0.270	-2.151	0.0041	0.4752		/
(A–B–C)	C$_{2v}$	A: 0.932	-0.766	0.0009	0.7370	0.094	-25.2
		B: 0.172	-2.390	0.0038	0.1490	0.032	-2.9
		C: -1.006	-2.921	0.0079	0.0444	0.021	36.7
		peri: 0.008	-2.833	0.0052	0.3499		/
(A–B–C)	C$_s$	A: 0.573	-1.042	0.0020	0.3246	0.046	-19.4
		B: 0.828	-1.049	0.0009	0.6487	0.074	-19.1
		C: -1.949	-6.442	0.0154	0.0227	0.011	61.9
		peri: -0.138	-3.145	0.0063	0.3216		/
(A–B–C–D)	C$_{2v}$	A: 0.893	-0.750	0.0005	0.6753	0.086	-26.2
		B: 0.377	-1.780	0.0027	0.2307	0.040	-10.4
		C: -0.820	-0.967	0.0044	0.0468	0.017	30.2
		D: 0.915	-1.212	0.0003	0.7184	0.105	-16.6
		peri: 0.401	-1.925	0.0034	0.4707		/
(A / B–C–D)	C$_s$	A: 0.708	-0.886	0.0014	0.4155	0.059	-23.5
		B: 0.876	-0.627	0.0006	0.6230	0.069	-21.0
		C: -1.033	-2.289	0.0082	0.0291	0.017	45.5
		D: 0.799	-1.604	0.0009	0.5446	0.099	-9.1
		peri: 0.364	-1.799	0.0035	0.4183		/
(A–B–C–D)	C$_{2v}$	A: 0.798	-0.866	0.0009	0.4674	0.063	-26.4
		B: 0.765	-0.493	0.0009	0.4488	0.052	-25.6
		C: -0.086	-2.735	0.0049	0.1246	0.020	-0.3
		D: -0.836	-2.351	0.0066	0.0679	0.023	30.4
		peri: 0.265	-2.406	0.0042	0.3114		/
(A–B–C / D)	C$_s$	A: 0.522	-1.183	0.0023	0.2761	0.041	-19.3
		B: 0.682	-0.297	0.0010	0.4286	0.042	-28.5
		C: 0.791	-0.899	0.0012	0.5944	0.063	-23.4
		D: -2.201	-7.437	0.0174	0.0234	0.009	68.5
		peri: 0.046	-2.649	0.0053	0.3721		/
(A / B–C–D)	C$_s$	A: 0.849	-0.852	0.0007	0.5578	0.076	-27.9
		B: 0.686	-0.314	0.0011	0.3904	0.046	-23.0
		C: 0.352	-2.222	0.0031	0.1929	0.045	-3.4
		D: -1.113	-3.370	0.0090	0.0319	0.019	41.8
		peri: 0.163	-2.335	0.0046	0.3364		/
(B–C / D, A)	C$_s$	A: 0.938	-0.859	0.0003	0.7170	0.093	-27.4
		B: 0.219	-0.684	0.0027	0.1874	0.019	-10.5
		C: 0.768	-1.401	0.0012	0.5534	0.077	-14.2
		D: -1.704	-5.572	0.0137	0.0230	0.013	57.0
		peri: 0.055	-2.603	0.0052	0.3554		/
(A / B–C / D)	C$_s$	A: 0.949	-0.870	0.0002	0.7204	0.093	-27.9
		B: 0.274	-0.585	0.0025	0.1925	0.019	-10.1
		C: 0.773	-1.327	0.0011	0.5462	0.078	-14.1
		D: -1.726	-5.558	0.0135	0.0243	0.014	58.7
		peri: 0.076	-2.567	0.0050	0.3610		/
(C / B–A / A)	C$_{2v}$	A: 0.812	-0.785	0.0009	0.5434	0.071	-26.7
		B: 0.620	-0.484	0.0021	0.4249	0.037	-21.1
		C: -2.495	-8.670	0.0200	0.0243	0.007	64.5
		peri: -0.007	-2.564	0.0055	0.4160		/

Table S4. Symmetry point group (PG), spin density at carbon atoms (SD), HOMA, HOMER, Shannon aromaticity index (SA), electron density of delocalized bond per atom (EDDB$_P$, in e), multicenter index (MCI) and NICS(1)$_{zz}$ (in

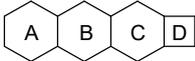ppm) calculated for T_1 state of given polycycles at the UCAM-B3LYP/6-311+G(d,p) (normal font) and M06-2X/6-311+G(d,p) (*italic*) levels of theory. ″Peri″ means molecular perimeter. NICS is calculated only with UCAM-B3LYP.

Compound	PG	SD	HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$
A B	C_{2v}	A: 0.89	0.764	-0.568	0.0006	0.4534	0.044	-23.6
		0.91	*0.730*	*-0.396*	*0.0006*	*0.4534*	*0.042*	
		B: 1.44	0.037	0.428	0.0008	0.1765	0.089	-25.2
		1.42	*0.020*	*0.409*	*0.0007*	*0.1670*	*0.089*	
		peri: 1.90	0.615	-0.400	0.0015	0.5078		/
		1.90	*0.618*	*-0.244*	*0.0013*	*0.5177*		
A B A	D_{2h}	A: 0.97	0.515	-0.918	0.0016	0.2795	0.027	-19.4
		0.97	*0.490*	*-0.761*	*0.0015*	*0.2849*	*0.026*	
		B: 1.08	-0.117	0.274	0.0001	0.0764	0.057	-35.6
		1.05	*-0.166*	*0.180*	*0.0002*	*0.0691*	*0.055*	
		peri: 1.95	0.776	-0.730	0.0012	0.4386		/
		1.95	*0.771*	*-0.546*	*0.0011*	*0.4522*		
A B C	C_{2v}	A: 0.33	0.662	-0.894	0.0015	0.4159	0.055	-25.1
		0.35	*0.627*	*-0.732*	*0.0016*	*0.4056*	*0.053*	
		B: 0.69	0.522	-0.544	0.0012	0.3621	0.026	-28.8
		0.71	*0.471*	*-0.429*	*0.0012*	*0.3598*	*0.024*	
		C: 1.32	-0.375	-0.491	0.0020	0.0767	0.057	-23.2
		1.30	*-0.341*	*-0.407*	*0.0012*	*0.0753*	*0.060*	
		peri: 1.90	0.545	-1.062	0.0022	0.4771		/
		1.91	*0.571*	*-0.829*	*0.0018*	*0.4838*		
A B C (C above)	C_s	A: 0.27	0.906	-0.682	0.0004	0.6696	0.081	-26.9
		0.29	*0.887*	*-0.477*	*0.0004*	*0.6598*	*0.079*	
		B: 0.90	0.571	-0.008	0.0008	0.3073	0.019	-12.7
		0.90	*0.539*	*0.079*	*0.0008*	*0.3153*	*0.019*	
		C: 1.43	0.312	0.871	0.0001	0.3016	0.110	-26.0
		1.41	*0.282*	*0.841*	*0.0001*	*0.2892*	*0.107*	
		peri: 1.92	0.737	-0.345	0.0011	0.5419		/
		1.92	*0.734*	*-0.199*	*0.0010*	*0.5510*		
A B C D	C_s/C_{2v}	A: 0.35	0.542	-1.035	0.0021	0.3385		-4.7
		0.39	*0.715*	*-0.447*	*0.0010*	*0.3717*	*0.060*	
		B: 0.70	0.427	-0.706	0.0016	0.3159	*0.044*	18.1
		0.72	*0.470*	*-0.006*	*0.0009*	*0.3116*	0.012	
		C: 0.96	-0.342	-0.201	0.0006	0.0752	*0.018*	15.9
		0.93	*0.126*	*0.918*	*0.0003*	*0.0608*	0.041	
		D: 1.11	0.265	-1.370	0.0003	0.2196	*0.044*	11.9
		1.06	*0.770*	*-0.197*	*0.0003*	*0.3071*	0.031	
		peri: 1.95	0.718	-1.064	0.0015	0.4118	*0.020*	/
		1.95	*0.787*	*-0.294*	*0.0008*	*0.5248*		
A (B C D)	C_s	A: 0.33	0.916	-0.682	0.0003	0.7101	0.083	-22.0
		0.33	*0.905*	*-0.469*	*0.0003*	*0.7132*	*0.082*	
		B: 1.02	0.258	-0.419	0.0016	0.2562	0.011	3.5
		0.98	*0.279*	*-0.268*	*0.0014*	*0.2624*	*0.012*	
		C: 1.02	-0.104	0.440	0.0003	0.1763	0.050	-24.5
		1.00	*-0.100*	*0.459*	*0.0002*	*0.1642*	*0.052*	
		D: 0.68	0.801	-0.585	0.0005	0.5067	0.054	-27.3
		0.72	*0.748*	*-0.418*	*0.0006*	*0.4789*	*0.049*	
		peri: 1.95	0.801	-0.632	0.0010	0.5724		/
		1.95	*0.800*	*-0.438*	*0.0009*	*0.5800*		
A B C D	C_{2v}[a]	A: 0.63	0.758	-0.736	0.0011	0.3758	0.053	8.6
		0.59	*0.792*	*-0.552*	*0.0007*	*0.4402*	*0.059*	
		B: 0.99	0.536	0.720	0.0003	0.2992	0.013	32.5
		1.06	*0.484*	*0.815*	*0.0002*	*0.3126*	*0.012*	
		C: 0.37	0.755	-1.324	0.0011	0.4642	0.066	0.1
		0.39	*0.773*	*-1.016*	*0.0010*	*0.4953*	*0.066*	
		D: 0.20	-1.452	-4.630	0.0117	0.0269	0.017	33.7
		0.20	*-1.461*	*-4.588*	*0.0117*	*0.0263*	*0.017*	
		peri: 1.90	0.145	-1.831	0.0043	0.3379		/
		1.01	*0.139*	*-1.627*	*0.0041*	*0.3561*		

Structure	PG							
(A–B–C, D)	C_s	A: 0.13	0.821	-0.800	0.0008	0.5086	0.067	-27.2
		0.14	*0.797*	*-0.611*	*0.0008*	*0.5005*	*0.066*	
		B: 0.27	0.709	-0.382	0.0010	0.4174	0.044	-25.2
		0.28	*0.690*	*-0.223*	*0.0010*	*0.4239*	*0.043*	
		C: 0.90	0.413	-0.091	0.0012	0.2867	0.013	-3.8
		0.91	*0.396*	*-0.011*	*0.0011*	*0.2930*	*0.014*	
		D: 1.35	0.335	0.844	0.0001	0.3218	0.105	-21.7
		1.32	*0.310*	*0.841*	*0.0001*	*0.3172*	*0.103*	
		peri: 1.92	0.756	-0.548	0.0011	0.4940		/
		1.92	*0.752*	*-0.383*	*0.0010*	*0.5045*		
(A, B–C–D)	C_s	A: 0.09	0.933	-0.840	0.0003	0.6960	0.089	-27.6
		0.10	*0.923*	*-0.623*	*0.0003*	*0.6954*	*0.089*	
		B: 0.34	0.314	-0.502	0.0023	0.2377	0.022	-13.0
		0.36	*0.279*	*-0.393*	*0.0022*	*0.2453*	*0.022*	
		C: 0.75	0.605	-0.513	0.0010	0.3814	0.029	-26.2
		0.77	*0.554*	*-0.389*	*0.0010*	*0.3748*	*0.026*	
		D: 1.33	-0.945	0.096	0.0012	0.1085	0.071	-25.8
		1.31	*-0.087*	*0.115*	*0.0010*	*0.1047*	*0.072*	
		peri: 1.91	0.591	-0.905	0.0019	0.4750		/
		1.92	*0.598*	*-0.706*	*0.0017*	*0.4839*		
(B–C, D / A)	C_s	A: 0.08	0.864	-0.824	0.0006	0.5920	0.079	-28.0
		0.09	*0.853*	*-0.621*	*0.0006*	*0.5966*	*0.079*	
		B: 0.23	0.626	-0.289	0.0013	0.3458	0.039	-21.6
		0.25	*0.594*	*-0.148*	*0.0013*	*0.3494*	*0.038*	
		C: 0.88	0.672	-0.079	0.0007	0.3475	0.026	-16.1
		0.89	*0.641*	*0.044*	*0.0006*	*0.3541*	*0.025*	
		D: 1.44	0.259	0.775	0.0003	0.2490	0.104	-26.2
		1.41	*0.233*	*0.744*	*0.0003*	*0.2349*	*0.102*	
		peri: 1.92	0.664	-0.519	0.0015	0.4751		/
		1.92	*0.659*	*-0.367*	*0.0013*	*0.4838*		
(A / B–C, D)	C_s	A: 0.07	0.885	-0.830	0.0009	0.7658	0.079	-28.8
		0.08	*0.877*	*-0.624*	*0.0005*	*0.6031*	*0.079*	
		B: 0.25	0.684	-0.176	0.0010	0.3694	0.039	-21.5
		0.27	*0.660*	*-0.032*	*0.0010*	*0.3721*	*0.038*	
		C: 0.88	0.625	-0.152	0.0008	0.3364	0.025	-16.5
		0.88	*0.594*	*-0.040*	*0.0008*	*0.3435*	*0.024*	
		D: 1.42	0.248	0.803	0.0001	0.2503	0.104	-26.3
		1.39	*0.214*	*0.755*	*0.0001*	*0.2368*	*0.101*	
		peri: 1.91	0.700	-0.463	0.0013	0.4879		/
		1.92	*0.697*	*-0.306*	*0.0011*	*0.4967*		
(C / B–A / A)	C_{2v}	A: 0.22	0.909	-0.723	0.0004	0.6953	0.084	-22.8
		0.23	*0.894*	*-0.527*	*0.0004*	*0.6898*	*0.084*	
		B: 0.82	0.296	0.389	0.0010	0.2249	0.009	-4.1
		0.82	*0.265*	*0.431*	*0.0009*	*0.2291*	*0.010*	
		C: 1.48	0.430	0.988	0.0001	0.3665	0.122	-20.4
		1.46	*0.410*	*0.984*	*0.0000*	*0.3560*	*0.119*	
		peri: 1.92	0.701	-0.499	0.0013	0.5778		/
		1.93	*0.694*	*-0.346*	*0.0012*	*0.5800*		

[a] i 485.8 cm^{-1} (bond lengths).

Table S5. Symmetry point group (PG), HOMA, HOMER, Shannon aromaticity index (SA), electron density of delocalized bond per atom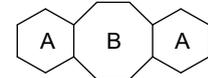 (EDDB$_P$, in e), multicenter index (MCI) and NICS(1)$_{zz}$ (in ppm) calculated for S$_0$ state of given polycycles at the CAM-B3LYP/6-311+G(d,p) level of theory. ″Peri″ means molecular perimeter.

Compound	PG	HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$
(A–B)	C_{2v}[a]	A: 0.954	-0.876	0.0003	0.7463	0.101	-10.1
		B: -0.164	-3.189	0.0060	0.0578	0.002	45.2
		peri: 0.234	-2.660	0.0042	0.3154		/
(A–B–A)	D_{2h}[b]	A: 0.963	-0.886	0.0002	0.7752	0.100	-16.4
		B: -0.094	-2.055	0.0045	0.0734	0.002	30.3
		peri: 0.455	-1.761	0.0028	0.4736		/

Compound	PG	SD	HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$
rings A, B, C	C$_{2v}$[c]	A: 0.895	-0.868		0.0005	0.5798	0.076	-22.9
		B: 0.759	-0.486		0.0011	0.3276	0.047	-8.6
		C: -0.093	-2.769		0.0055	0.0823	0.003	33.2
		peri: 0.442	-2.030		0.0031	0.3000		/
rings A, B, C	C$_s$[d]	A: 0.756	-0.927		0.0012	0.4781	0.067	-25.9
		B: 0.674	-0.547		0.0013	0.5213	0.060	-16.5
		C: -0.206	-3.498		0.0063	0.0449	0.002	57.2
		peri: 0.232	-2.322		0.0042	0.2898		/
rings A, B, C, D	C$_{2v}$[e]	A: 0.865	-0.866		0.0006	0.5350	0.072	-24.4
		B: 0.821	-0.401		0.0007	0.3818	0.051	-15.4
		C: -0.082	-1.810		0.0042	0.0872	0.002	24.1
		D: 0.956	-0.873		0.0002	0.7875	0.102	-18.7
		peri: 0.544	-1.524		0.0024	0.4166		/
rings A, B, C, D	C$_s$[f]	A: 0.785	-0.905		0.0011	0.5056	0.070	-26.8
		B: 0.648	-0.621		0.0015	0.4699	0.056	-19.6
		C: -0.076	-2.189		0.0045	0.0580	0.002	36.8
		D: 0.974	-0.924		0.0001	0.7935	0.104	-14.0
		peri: 0.432	-1.597		0.0028	0.4127		/
rings A, B, C, D	C$_{2v}$[g]	A: 0.699	-0.949		0.0014	0.3900	0.056	-24.1
		B: 0.863	-0.333		0.0004	0.5184	0.053	-26.7
		C: 0.578	-0.630		0.0019	0.2256	0.031	-6.9
		D: -0.054	-2.583		0.0052	0.1013	0.004	26.9
		peri: 0.526	-1.835		0.0026	0.2968		/
rings A, B, C, D	C$_s$[h]	A: 0.656	-1.055		0.0017	0.3299	0.049	-23.4
		B: 0.816	-0.206		0.0005	0.5293	0.051	-32.2
		C: 0.460	-0.844		0.0023	0.3397	0.042	-17.7
		D: -0.225	-3.663		0.0065	0.0429	0.001	62.2
		peri: 0.292	-2.125		0.0037	0.2880		/
rings A, B, C, D	C$_s$[i]	A: 0.898	-0.844		0.0005	0.6313	0.083	-28.2
		B: 0.592	-0.502		0.0016	0.2832	0.034	-18.1
		C: 0.869	-0.453		0.0006	0.4753	0.064	-8.1
		D: -0.098	-2.879		0.0055	0.0693	0.003	38.7
		peri: 0.442	-1.811		0.0029	0.3178		/
rings A, B, C, D	C$_s$[j]	A: 0.923	-0.910		0.0004	0.6558	0.086	-28.8
		B: 0.433	-0.529		0.0021	0.2405	0.028	-18.0
		C: 0.771	-0.461		0.0010	0.6467	0.073	-13.4
		D: -0.191	-3.367		0.0061	0.0481	0.002	53.5
		peri: 0.310	-1.997		0.0036	0.3226		/
rings A, B, C, D	C$_1$[k]	A: 0.892	-0.814		0.0005	0.6699	0.087	-28.7
		B: 0.415	-0.623		0.0023	0.2585	0.031	-18.3
		C: 0.813	-0.578		0.0008	0.5964	0.076	-28.7
		D: -0.311	-3.975		0.0067	0.0443	0.001	8.5
		peri: 0.258	-2.225		0.0038	0.3226		/
rings A, B, C, D	C$_{2v}$[l]	A: 0.859	-0.975		0.0008	0.6287	0.084	-28.5
		B: 0.197	-0.117		0.0018	0.2215	0.026	-14.2
		C: 0.859	-0.975		0.0008	0.6287	0.084	-28.5
		D: -0.246	-3.782		0.0065	0.0410	0.001	60.1
		peri: 0.214	-1.997		0.0038	0.3544		/

[a] *i* 108.1 cm^{-1} (COT out-of-plane (oop)). [b] *i* 59.1 cm^{-1} (oop). [c] *i* 87.3 cm^{-1} (COT oop). [d] *i* 159.9 cm^{-1} (COT oop), 43.0 cm^{-1} (HH steric). [e] *i* 43.4 cm^{-1} (COT oop). [f] *i* 101.9 cm^{-1}, 28.7 cm^{-1} (HH steric). [g] *i* 77.9 cm^{-1} (COT oop). [h] *i* 163.4 cm^{-1} (COT oop), 41.8 (oop). [i] *i* 91.5 cm^{-1} (COT oop). [j] *i* 166.5 cm^{-1} (COT oop), 50.0 (oop). [k] COT ring is nonplanar. [l] *i* 222.8 cm^{-1} (COT oop), 148.0 (HH steric), 43.5 (oop).

Table S6. Symmetry point group (PG), spin density at carbon atoms (SD), HOMA, HOMER, Shannon aromaticity index (SA), electron density of delocalized bond per atom (EDDB$_P$, in e), multicenter index (MCI) and NICS(1)$_{zz}$ (in ppm) calculated for T$_1$ state of given polycycles at the UCAM-B3LYP/6-311+G(d,p) (normal font) and M06-2X/6-311+G(d,p) (*italic*) levels of theory. "Peri" means molecular perimeter. NICS is calculated only with UCAM-B3LYP.

Compound	PG	SD	HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$

Structure	Symmetry							
A–B (6,7 rings)	C_{2v}	A: 0.48	0.745	-0.764	0.0012	0.5422	0.066	-30.1
		0.50	*0.704*	*-0.587*	*0.0013*	*0.5215*	*0.063*	
		B: 1.63	0.748	-0.273	0.0008	0.5068	0.026	-25.4
		1.63	*0.742*	*-0.121*	*0.0008*	*0.5271*	*0.027*	
		peri: 1.90	0.808	-0.731	0.0009	0.5627		/
		1.91	*0.805*	*-0.537*	*0.0009*	*0.5779*		
A–B–A	D_{2h}	A: 0.54	0.541	-1.082	0.0022	0.3403	0.045	-25.1
		0.55	*0.529*	*-0.877*	*0.0021*	*0.3463*	*0.045*	
		B: 1.45	0.738	0.165	0.0004	0.4955	0.021	-34.2
		1.43	*0.698*	*0.264*	*0.0004*	*0.4888*	*0.020*	
		peri: 1.92	0.737	-0.962	0.0013	0.4809		/
		1.93	*0.733*	*-0.743*	*0.0013*	*0.4918*		
A–B–C	C_{2v}	A: 0.20	0.773	-0.899	0.0011	0.4199	0.058	-28.0
		0.21	*0.741*	*-0.714*	*0.0012*	*0.4050*	*0.055*	
		B: 0.41	0.730	-0.079	0.0009	0.4181	0.039	-33.8
		0.43	*0.682*	*0.025*	*0.0010*	*0.4138*	*0.037*	
		C: 1.49	0.594	-0.452	0.0015	0.3862	0.015	-16.2
		1.50	*0.595*	*-0.311*	*0.0014*	*0.4073*	*0.016*	
		peri: 1.90	0.799	-0.750	0.0010	0.4790		/
		1.91	*0.797*	*-0.567*	*0.0009*	*0.4976*		
A–B–C (angular, C on top)	$C_s{}^{a}$	A: 0.13	0.892	-0.848	0.0005	0.6589	0.085	-28.9
		0.14	*0.878*	*-0.629*	*0.0005*	*0.6589*	*0.085*	
		B: 0.49	0.258	-0.715	0.0027	0.2954	0.028	-18.2
		0.50	*0.218*	*-0.598*	*0.0027*	*0.3018*	*0.027*	
		C: 1.67	0.826	-0.277	0.0006	0.6054	0.035	-29.3
		1.65	*0.809*	*-0.126*	*0.0006*	*0.6159*	*0.036*	
		peri: 1.90	0.691	-0.922	0.0015	0.5527		/
		1.91	*0.685*	*-0.735*	*0.0015*	*0.5643*		
A–B–C–D	C_s/C_{2v}	A: 0.21	0.732	-0.865	0.0012	0.3860		-23.8
		0.22	*0.625*	*-0.845*	*0.0017*	*0.3193*	*0.051*	
		B: 0.44	0.658	-0.129	0.0011	0.3780	0.045	-28.9
		0.44	*0.659*	*-0.047*	*0.0011*	*0.3917*	*0.032*	
		C: 1.30	0.486	-0.325	0.0016	0.2668	*0.034*	-20.4
		1.34	*0.603*	*0.153*	*0.0007*	*0.4247*	0.011	
		D: 0.54	0.493	-1.090	0.0024	0.3341	*0.015*	-16.2
		0.58	*0.335*	*-1.210*	*0.0031*	*0.2502*	0.039	
		peri: 1.92	0.713	-0.989	0.0015	0.4025	*0.034*	/
		1.93	*0.735*	*-0.777*	*0.0013*	*0.4752*		
A–B–C–D (angular, A on top)	$C_s{}^{b}$	A: 0.15	0.943	-0.844	0.0003	0.7313	0.094	-26.4
		0.15	*0.925*	*-0.613*	*0.0003*	*0.7195*	*0.092*	
		B: 0.60	0.004	-0.999	0.0035	0.2095	0.016	-5.9
		0.58	*0.022*	*-0.843*	*0.0032*	*0.2264*	*0.017*	
		C: 1.43	0.696	0.024	0.0006	0.4638	0.020	-27.8
		1.42	*0.689*	*0.203*	*0.0005*	*0.4828*	*0.021*	
		D: 0.45	0.745	-0.833	0.0012	0.4843	0.061	-29.2
		0.48	*0.699*	*-0.659*	*0.0013*	*0.4554*	*0.057*	
		peri: 1.93	0.676	-0.986	0.0016	0.5211		/
		1.93	*0.670*	*-0.774*	*0.0015*	*0.5271*		
A–B–C–D	$C_{2v}/C_s{}^{c}$	A: 0.09	0.629	-1.023	0.0017	0.3371	0.048	-25.5
		0.10	*0.590*	*-0.873*	*0.0018*	*0.3272*	*0.047*	
		B: 0.18	0.830	-0.223	0.0004	0.4840	0.046	-36.6
		0.20	*0.789*	*-0.072*	*0.0005*	*0.4641*	*0.044*	
		C: 0.38	0.584	-0.094	0.0013	0.3120	0.027	-29.7
		0.40	*0.548*	*0.016*	*0.0013*	*0.3331*	*0.028*	
		D: 1.39	0.492	-0.643	0.0019	0.3291	0.011	-8.3
		1.41	*0.498*	*-0.498*	*0.0018*	*0.3580*	*0.013*	
		peri: 1.90	0.793	-0.830	0.0011	0.4706		/
		1.91	*0.791*	*-0.639*	*0.0010*	*0.4846*		
A–B–C–D (angular, D on top)	$C_s{}^{d}$	A: 0.05	0.772	-0.917	0.0011	0.4240	0.060	-27.0
		0.06	*0.758*	*-0.726*	*0.0011*	*0.4279*	*0.060*	
		B: 0.12	0.839	-0.298	0.0005	0.5066	0.054	-31.2
		0.13	*0.811*	*-0.134*	*0.0005*	*0.5015*	*0.053*	
		C: 0.50	0.047	-0.869	0.0033	0.2481	0.018	-9.3

Compound (ring labels)	PG		HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$
		0.52	*0.022*	*-0.746*	*0.0032*	*0.2602*	*0.018*	
		D: 1.65	0.849	-0.291	0.0005	0.6414	0.038	-29.2
		1.64	*0.829*	*-0.145*	*0.0005*	*0.6445*	*0.038*	
		peri: 1.91	0.686	-1.001	0.0015	0.4994		/
		1.91	*0.682*	*-0.814*	*0.0015*	*0.5079*		
A–B–C–D (7-ring at D)	C$_s$	A: 0.05	0.929	-0.846	0.0003	0.6914	0.089	-28.6
		0.06	*0.921*	*-0.629*	*0.0003*	*0.6950*	*0.089*	
		B: 0.18	0.445	-0.509	0.0020	0.2252	0.024	-16.0
		0.20	*0.402*	*-0.394*	*0.0020*	*0.2281*	*0.023*	
		C: 0.42	0.779	-0.151	0.0008	0.4877	0.047	-32.6
		0.45	*0.724*	*-0.034*	*0.0009*	*0.4676*	*0.044*	
		D: 1.54	0.675	-0.351	0.0011	0.4449	0.019	-20.5
		1.53	*0.675*	*-0.205*	*0.0010*	*0.4691*	*0.021*	
		peri: 1.90	0.745	-0.789	0.0012	0.4975		/
		1.91	*0.740*	*-0.611*	*0.0011*	*0.5079*		
A–B–C–D (7-ring at D)	C$_s$ [e]	A: 0.03	0.892	-0.890	0.0005	0.6012	0.080	-28.3
		0.04	*0.880*	*-0.680*	*0.0005*	*0.6007*	*0.080*	
		B: 0.13	0.601	-0.433	0.0015	0.3163	0.039	-21.6
		0.13	*0.574*	*-0.285*	*0.0015*	*0.3245*	*0.039*	
		C: 0.48	0.405	-0.604	0.0010	0.3699	0.037	-21.9
		0.50	*0.363*	*-0.460*	*0.0023*	*0.3694*	*0.036*	
		D: 1.65	0.800	-0.283	0.0009	0.5697	0.032	-27.8
		1.64	*0.788*	*-0.127*	*0.0006*	*0.5868*	*0.033*	
		peri: 1.90	0.668	-0.841	0.0016	0.5105		/
		1.91	*0.659*	*-0.658*	*0.0015*	*0.5222*		
A–B–C–D (7-ring at D)	C$_1$ [f]	A: 0.05	0.864	-0.807	0.0006	0.6013		-30.8
		0.06	*0.849*	*-0.606*	*0.0006*	*0.5977*	0.079	
		B: 0.14	0.599	-0.467	0.0016	0.3361	*0.079*	-22.3
		0.15	*0.589*	*-0.296*	*0.0015*	*0.3472*	0.040	
		C: 0.49	0.498	-0.421	0.0018	0.3487	*0.040*	-21.6
		0.51	*0.470*	*-0.257*	*0.0018*	*0.3472*	0.035	
		D: 1.62	0.827	-0.246	0.0005	0.5681	*0.034*	-24.8
		1.60	*0.814*	*-0.102*	*0.0005*	*0.5765*	0.032	
		peri: 1.90	0.713	-0.762	0.0013	0.5153	*0.032*	/
		1.90	*0.711*	*-0.566*	*0.0012*	*0.5242*		
A/B/C/D (7-ring at D)	C$_{2v}$ [g]	A: 0.10	0.910	-0.973	0.0005	0.7111	0.094	-24.6
		0.11	*0.898*	*-0.750*	*0.0005*	*0.7078*	*0.093*	
		B: 0.47	-0.220	-0.170	0.0018	0.1729	0.012	-6.2
		0.48	*-0.264*	*-0.131*	*0.0017*	*0.1854*	*0.012*	
		C: 0.10	0.910	-0.973	0.0005	0.7111	0.094	-24.6
		0.11	*0.898*	*-0.750*	*0.0005*	*0.7078*	*0.093*	
		D: 1.70	0.861	-0.304	0.0005	0.6414	0.040	-28.0
		1.69	*0.842*	*-0.148*	*0.0005*	*0.6441*	*0.040*	
		peri: 1.91	0.599	-0.913	0.0018	0.5779		/
		1.91	*0.589*	*-0.738*	*0.0017*	*0.5836*		

[a] *i* 80.5/*92.1* cm^{-1} (HH steric). [b] *i* 67.7/*75.9* cm^{-1} (HH steric). [c] *i* 32.6 cm^{-1} (out-of-plane). [d] *i* 79.5/*95.9* cm^{-1} (HH steric). [e] *i* 95.3/*113.6* cm^{-1} (HH steric). [f] The system is nonplanar. [g] *i* 152.8, 125.2/*165.5, 137.1, 29.1* cm^{-1} (HH steric).

Table S7. Symmetry point group (PG), HOMA, HOMER, Shannon aromaticity index (SA), electron density of delocalized bond per atom (EDDB$_P$, in e), multicenter index (MCI) and NICS(1)$_{zz}$ (in ppm) calculated for S$_0$ state of given polycycles at the CAM-B3LYP/6-311+G(d,p) level of theory. ″Peri″ means molecular perimeter, ″peri-p″ perimeter of pentalene subunit.

Compound	PG	HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$
A–A	C$_{2h}$	A: -0.420	-3.268	0.0067	0.0605	0.021	48.6
		peri: -0.459	-4.229	0.0080	0.0434	-0.010	/
A–B–C	C$_s$	A: -0.279	-2.852	0.0057	0.0756	0.026	30.8
		B: -0.282	-1.502	0.0042	0.0683	0.013	32.0
		C: 0.928	-1.112	0.0003	0.7175	0.102	-13.2
		peri-p: -0.202	-2.762	0.0059	0.0585	-0.001	/
		peri: 0.202	-2.508	0.0043	0.3039		/

Structure	Symmetry	Label					
(structure 1)	C_{2h}	A: 0.950	-1.016	0.0002	0.7558	0.102	-17.1
		B: -0.225	-1.419	0.0039	0.0794	0.016	22.4
		peri-p: -0.095	-1.759	0.0045	0.0682	0.001	/
		peri: 0.468	-1.793	0.0028	0.4541		/
(structure 2)	$C_s^{\,a}$	A: 0.915	-1.071	0.0003	0.6879	0.096	2.4
		B: -0.075	-0.965	0.0034	0.0919	0.016	62.7
		C: -0.098	-1.838	0.0039	0.0949	0.024	70.1
		D: 0.044	-1.906	0.0041	0.1402	0.019	26.1
		peri-p: -0.066	-1.922	0.0044	0.0725	-0.001	/
		peri: 0.461	-1.943	0.0030	0.2803		/
(structure 3)	C_s	A: -0.176	-2.542	0.0051	0.0841	0.029	22.3
		B: -0.296	-1.222	0.0036	0.0950	0.012	23.7
		C: 0.567	-1.187	0.0019	0.2995	0.045	-10.8
		D: 0.887	-0.773	0.0005	0.6270	0.080	-24.8
		peri-p: -0.119	-2.354	0.0052	0.0836	0.001	/
		peri: 0.372	-2.119	0.0034	0.3054		/
(structure 4)	C_s	A: -0.316	-2.982	0.0060	0.0707	0.025	40.8
		B: -0.251	-1.825	0.0048	0.0643	0.015	43.8
		C: 0.876	-0.404	0.0004	0.3576	0.062	-18.7
		D: 0.763	-0.862	0.0011	0.2099	0.063	-24.1
		peri-p: -0.241	-3.092	0.0064	0.0522	-0.003	/
		peri: 0.298	-2.036	0.0037	0.298		/
(structure 5)	C_s	A: 0.953	-0.974	0.0001	0.7643	0.100	-18.8
		B: -0.175	-1.304	0.0036	0.0866	0.016	17.5
		C: -0.269	-1.212	0.0035	0.1043	0.013	17.2
		D: 0.611	-1.060	0.0017	0.3344	0.048	-15.2
		E: 0.868	-0.780	0.0006	0.5934	0.077	-25.7
		peri-p: -0.082	-1.546	0.0042	0.0877	0.001	/
		peri: 0.526	-1.697	0.0025	0.4167		/
(structure 6)	C_s	A: 0.909	-0.998	0.0003	0.6816	0.093	33.4
		B: 0.117	-0.508	0.0026	0.1270	0.019	124.2
		C: 0.079	-1.181	0.0029	0.1220	0.026	143.8
		D: 0.191	-1.105	0.0028	0.1866	0.019	73.4
		E: 0.228	-1.646	0.0036	0.1825	0.026	24.5
		peri-p: 0.075	-1.294	0.0034	0.0961	-0.002	/
		peri: 0.582	-1.597	0.0023	0.3092		/
(structure 7)	C_s	A: -0.117	-2.362	0.0047	0.0892	0.031	17.3
		B: -0.315	-1.165	0.0035	0.1110	0.012	18.9
		C: 0.321	-1.516	0.0030	0.2052	0.029	-8.2
		D: 0.819	-0.314	0.0006	0.5075	0.053	-27.7
		E: 0.735	-0.917	0.0012	0.4091	0.058	-25.3
		peri-p: -0.082	-2.189	0.0049	0.0993	0.002	/
		peri: 0.454	-1.946	0.0030	0.2898		/
(structure 8)	C_s	A: -0.337	-3.034	0.0061	0.0690	0.024	45.3
		B: -0.255	-2.014	0.0051	0.0629	0.016	48.8
		C: 0.745	-0.457	0.0010	0.4181	0.046	-19.4
		D: 0.792	-0.240	0.0006	0.5098	0.049	-31.0
		E: 0.625	-1.049	0.0021	0.3256	0.048	-22.9
		peri-p: -0.265	-3.255	0.0067	0.0504	-0.004	/
		peri: 0.365	-1.856	0.0033	0.3043		/
(structure 9)	C_s	A: -0.210	-2.644	0.0053	0.0821	0.028	26.2
		B: -0.256	-1.265	0.0037	0.0852	0.013	28.1
		C: 0.721	-1.035	0.0012	0.4090	0.059	-10.9
		D: 0.594	-0.383	0.0015	0.3080	0.036	-19.6
		E: 0.887	-0.845	0.0005	0.6187	0.083	-28.1
		peri-p: -0.127	-2.462	0.0054	0.0740	0.001	/
		peri: 0.446	-1.848	0.0032	0.3171		/
(structure 10)	C_s	A: -0.294	-2.913	0.0059	0.0732	0.025	37.5
		B: -0.249	-1.696	0.0046	0.0650	0.015	40.1
		C: 0.920	-0.515	0.0002	0.6679	0.073	-16.2
		D: 0.431	-0.490	0.0020	0.2323	0.026	-15.8
		E: 0.920	-0.856	0.0004	0.6784	0.089	-28.2
		peri-p: -0.221	-2.962	0.0034	0.0552	-0.002	

| | | peri: 0.348 | -1.846 | 0.0034 | 0.3312 | | / |

a RHF → UHF instability.

Table S8. Symmetry point group (PG), spin density at carbon atoms (SD), HOMA, HOMER, Shannon aromaticity index (SA), electron density of delocalized bond per atom (EDDB$_P$, in e), multicenter index (MCI) and NICS(1)$_{zz}$ (in ppm) calculated for T$_1$ state of given polycycles at the UCAM-B3LYP/6-311+G(d,p) (normal font) and M06-2X/6-311+G(d,p) (*italic*) levels of theory. ″Peri″ means molecular perimeter. NICS is calculated only with UCAM-B3LYP.

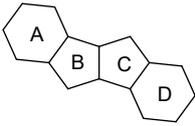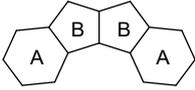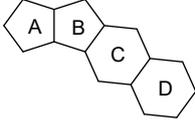| Compound	PG	SD	HOMA	HOMER	SA	EDDB$_P$	MCI	NICS(1)$_{zz}$
(A A)	D$_{2h}$	A: 1.15	0.487	-0.066	0.0007	0.4806	0.045	-30.5
		1.15	*0.432*	*-0.002*	*0.0007*	*0.4786*	*0.045*	
		peri: 1.90	0.892	0.086	0.0000	0.6333	0.052	/
		1.91	*0.862*	*0.235*	*0.0000*	*0.6916*	*0.053*	
(A B C)	C$_s$	A: 1.10	0.387	-0.404	0.0016	0.2982	0.048	-19.3
		1.10	*0.359*	*-0.290*	*0.0014*	*0.3207*	*0.048*	
		B: 0.93	0.370	0.610	0.0003	0.3045	0.026	-14.9
		0.94	*0.313*	*0.607*	*0.0003*	*0.3130*	*0.026*	
		C: 0.43	0.896	-0.654	0.0003	0.6682	0.076	-27.4
		0.45	*0.869*	*-0.447*	*0.0000*	*0.6506*	*0.073*	
		peri-p: 1.64	0.539	-0.016	0.0011	0.3936	0.016	/
		1.64	*0.538*	*0.116*	*0.0009*	*0.4158*	*0.017*	
		peri: 1.91	0.738	-0.504	0.0010	0.5470		/
		1.92	*0.743*	*-0.311*	*0.0009*	*0.5605*		
(A B C D)	C$_s$/C$_{2h}$ a	A: 0.55	0.609	-0.842	0.0015	0.3874	0.042	-15.0
		0.56	*0.646*	*-0.613*	*0.0012*	*0.4005*	*0.047*	
		B: 0.98	0.237	0.293	0.0010	0.2195	0.026	-20.4
		0.88	*0.251*	*0.132*	*0.0007*	*0.3095*	*0.026*	
		C: 0.81	0.416	0.148	0.0008	0.3232	0.032	-11.4
		0.88	*0.251*	*0.132*	*0.0007*	*0.3095*	*0.026*	
		D: 0.42	0.874	-0.627	0.0004	0.6163	0.069	-23.0
		0.56	*0.646*	*-0.613*	*0.0012*	*0.4005*	*0.047*	
		peri-p: 1.42	0.393	0.056	0.0012	0.2901	0.009	/
		1.41	*0.575*	*0.298*	*0.0004*	*0.4355*	*0.016*	
		peri: 1.93	0.762	-0.699	0.0011	0.4837		/
		1.94	*0.582*	*-0.439*	*0.0006*	*0.5317*		
(B B / A A)	C$_{2v}$	A: 0.37	0.916	-0.759	0.0002	0.6967	0.083	-25.7
		0.38	*0.901*	*-0.536*	*0.0002*	*0.6903*	*0.082*	
		B: 0.87	0.384	0.664	0.0004	0.2933	0.026	-6.0
		0.89	*0.343*	*0.683*	*0.0004*	*0.3036*	*0.027*	
		peri-p: 1.38	0.442	0.597	0.0005	0.3575	0.005	/
		1.39	*0.420*	*0.640*	*0.0005*	*0.3741*	*0.006*	
		peri: 1.92	0.777	-0.512	0.0009	0.6053		/
		1.92	*0.772*	*-0.330*	*0.0008*	*0.6142*		
(A B C D)	C$_s$	A: 1.06	0.346	-0.510	0.0020	0.2685	0.046	-10.3
		1.07	*0.327*	*-0.376*	*0.0018*	*0.2869*	*0.048*	
		B: 0.79	0.322	0.632	0.0003	0.2798	0.021	-7.2
		0.82	*0.275*	*0.636*	*0.0003*	*0.2794*	*0.022*	
		C: 0.36	0.596	-0.636	0.0014	0.3612	0.038	-24.7
		0.37	*0.582*	*-0.458*	*0.0013*	*0.3756*	*0.038*	
		D: 0.18	0.834	-0.762	0.0007	0.5449	0.070	-28.1
		0.19	*0.804*	*-0.575*	*0.0008*	*0.5270*	*0.068*	
		peri-p: 1.50	0.383	-0.155	0.0016	0.2207	0.008	/
		1.52	*0.373*	*-0.048*	*0.0014*	*0.3445*	*0.009*	
		peri: 1.91	0.689	-0.776	0.0015	0.4639		/
		1.92	*0.688*	*-0.582*	*0.0013*	*0.4765*		
(A B D / C)	C$_s$	A: 1.08	0.473	-0.239	0.0010	0.3883	0.049	-28.3
		1.07	0.441	-0.134	0.0009	0.4254	*0.049*	
		B: 0.99	0.419	0.452	0.0004	0.3465	0.030	-21.7
		0.98	0.349	0.0429	0.0004	0.3505	*0.030*	
		C: 0.44	0.697	-0.082	0.0008	0.3761	0.035	-21.2
		0.47	0.638	0.049	0.0009	0.3689	*0.032*	
		D: 0.14	0.871	-0.772	0.0006	0.5897	0.076	-27.9

		0.16	0.868	-0.565	0.0005	0.6048	*0.077*	
		peri-p: 1.69	0.723	0.116	0.0005	0.4946	0.027	/
		1.67	*0.728*	*0.272*	*0.0003*	*0.5282*	*0.029*	
		peri: 1.92	0.780	-0.468	0.0009	0.5160		/
		1.93	*0.785*	*-0.284*	*0.0007*	*0.5376*		
	C_s	A: 0.45	0.724	-0.665	0.0010	0.4782	0.049	-10.8
		0.49	*0.687*	*-0.553*	*0.0011*	*0.4633*	*0.049*	
		B: 0.92	0.232	0.197	0.0016	0.1998	0.025	-3.5
		0.92	*0.214*	*0.323*	*0.0013*	*0.2223*	*0.027*	
		C: 0.68	0.454	0.400	0.0008	0.3419	0.028	-0.8
		0.68	*0.405*	*0.407*	*0.0007*	*0.3318*	*0.029*	
		D: 0.33	0.572	-0.691	0.0015	0.3298	0.035	-18.8
		0.34	*0.558*	*-0.494*	*0.0014*	*0.3424*	*0.034*	
		E: 0.16	0.865	-0.728	0.0006	0.5831	0.074	-26.1
		0.17	*0.837*	*-0.530*	*0.0006*	*0.5640*	*0.071*	
		peri-p: 1.29	0.230	0.225	0.0011	0.2450	0.004	\
		1.28	*0.224*	*0.242*	*0.0011*	*0.2579*	*0.004*	
		peri: 1.92	0.716	-0.749	0.0013	0.4628		\
		1.93	*0.719*	*-0.574*	*0.0012*	*0.4719*		
	C_s	A: 0.35	0.917	-0.807	0.0002	0.6967	0.085	-24.0
		0.36	*0.904*	*-0.575*	*0.0002*	*0.6926*	*0.083*	
		B: 0.83	0.381	0.664	0.0005	0.2797	0.024	-1.0
		0.85	*0.344*	*0.700*	*0.0004*	*0.2933*	*0.026*	
		C: 0.74	0.332	0.687	0.0003	0.3032	0.021	-1.7
		0.77	*0.285*	*0.683*	*0.0003*	*0.3051*	*0.022*	
		D: 0.33	0.575	-0.728	0.0015	0.3313	0.037	-21.7
		0.34	*0.567*	*-0.544*	*0.0014*	*0.3497*	*0.038*	
		E: 0.17	0.863	-0.751	0.0007	0.5843	0.075	-28.1
		0.17	*0.838*	*-0.556*	*0.0006*	*0.5695*	*0.073*	
		peri-p: 1.24	0.375	0.598	0.0005	0.3366	0.003	/
		1.27	*0.350*	*0.628*	*0.0005*	*0.3499*	*0.004*	
		peri: 1.91	0.762	-0.679	0.0011	0.5341		/
		1.92	*0.757*	*-0.488*	*0.0010*	*0.5457*		
	C_s	A: 1.02	0.333	-0.546	0.0022	0.2567	0.045	-4.7
		1.04	*0.316*	*-0.406*	*0.0020*	*0.2755*	*0.047*	
		B: 0.70	0.278	0.480	0.0005	0.2565	0.020	-3.7
		0.74	*0.235*	*0.502*	*0.0005*	*0.2526*	*0.021*	
		C: 0.34	0.358	-0.887	0.0023	0.2517	0.024	-18.6
		0.35	*0.349*	*-0.728*	*0.0022*	*0.2659*	*0.025*	
		D: 0.17	0.799	-0.242	0.0006	0.4928	0.048	-32.2
		0.17	*0.766*	*-0.091*	*0.0006*	*0.4891*	*0.047*	
		E: 0.08	0.716	-0.925	0.0017	0.3938	0.056	-26.4
		0.09	*0.684*	*-0.758*	*0.0014*	*0.3861*	*0.054*	
		peri-p: 1.40	0.312	-0.288	0.0018	0.2919	0.005	/
		1.43	*0.300*	*-0.177*	*0.0017*	*0.3057*	*0.006*	
		peri: 1.91	0.689	-0.895	0.0015	0.4260		/
		1.92	*0.686*	*-0.699*	*0.0014*	*0.4410*		
	C_s	A: 1.03	0.534	-0.067	0.0006	0.4772	0.048	-31.8
		1.02	*0.485*	*-0.004*	*0.0006*	*0.4857*	*0.048*	
		B: 0.99	0.416	0.275	0.0005	0.3633	0.033	-25.5
		0.97	*0.342*	*0.256*	*0.0005*	*0.3562*	*0.032*	
		C: 0.48	0.481	-0.110	0.0014	0.2831	0.021	-11.4
		0.51	*0.428*	*-0.008*	*0.0014*	*0.2890*	*0.020*	
		D: 0.14	0.808	-0.309	0.0006	0.4900	0.051	-29.9
		0.15	*0.780*	*-0.171*	*0.0006*	*0.4832*	*0.050*	
		E: 0.07	0.752	-0.894	0.0012	0.4257	0.059	-26.7
		0.07	*0.741*	*-0.697*	*0.0011*	*0.4342*	*0.060*	
		peri-p: 1.66	0.810	0.189	0.0002	0.5825	0.033	/
		1.63	*0.782*	*0.296*	*0.0001*	*0.5865*	*0.034*	
		peri: 1.93	0.794	-0.604	0.0009	0.4955		/
		1.93	*0.786*	*-0.432*	*0.0008*	*0.5052*		

Structure	Sym	Label						
A–B–C–D–E (angular ring system)	C_s	A: 1.08	0.362	-0.479	0.0019	0.2769	0.047	-14.4
		1.08	*0.339*	*-0.354*	*0.0017*	*0.2957*	*0.048*	
		B: 0.84	0.369	0.684	0.0002	0.2921	0.023	-9.6
		0.86	*0.316*	*0.675*	*0.0002*	*0.2913*	*0.023*	
		C: 0.38	0.745	-0.498	0.0008	0.4677	0.048	-25.9
		0.39	*0.720*	*-0.311*	*0.0008*	*0.4708*	*0.047*	
		D: 0.16	0.507	-0.402	0.0017	0.2728	0.030	-19.0
		0.17	*0.461*	*-0.288*	*0.0018*	*0.2743*	*0.029*	
		E: 0.05	0.903	-0.840	0.0004	0.6494	0.085	-28.4
		0.05	*0.896*	*-0.631*	*0.0004*	*0.6561*	*0.086*	
		peri-p: 1.55	0.461	-0.076	0.0013	0.3574	0.011	/
		1.55	*0.456*	*0.035*	*0.0012*	*0.3724*	*0.012*	
		peri: 1.92	0.666	-0.770	0.0015	0.4568		/
		1.92	*0.663*	*-0.586*	*0.0014*	*0.4706*		
A–B–C–D–E (angular ring system)	C_s	A: 1.09	0.443	-0.302	0.0013	0.3444	0.049	-24.8
		1.08	*0.414*	*-0.193*	*0.0011*	*0.3766*	*0.049*	
		B: 0.96	0.416	0.518	0.0004	0.3251	0.028	-17.9
		0.96	*0.351*	*0.503*	*0.0004*	*0.3332*	*0.028*	
		C: 0.42	0.808	-0.129	0.0005	0.4821	0.047	-23.7
		0.45	*0.760*	*0.030*	*0.0005*	*0.4653*	*0.044*	
		D: 0.13	0.546	-0.407	0.0016	0.2815	0.033	-19.4
		0.14	*0.529*	*-0.276*	*0.0016*	*0.2944*	*0.034*	
		E: 0.04	0.896	-0.843	0.0005	0.6341	0.084	-28.3
		0.05	*0.881*	*-0.633*	*0.0005*	*0.6304*	*0.083*	
		peri-p: 1.67	0.665	0.052	0.0008	0.4451	0.022	/
		1.65	*0.667*	*0.211*	*0.0006*	*0.4768*	*0.024*	
		peri: 1.92	0.710	-0.588	0.0012	0.4792		/
		1.93	*0.711*	*-0.403*	*0.0011*	*0.4947*		
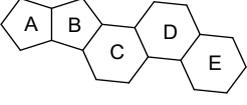
[a] *i 416.3* cm^{-1} (bond lengths).

Correlations for polybenzenoid compounds (T_1)
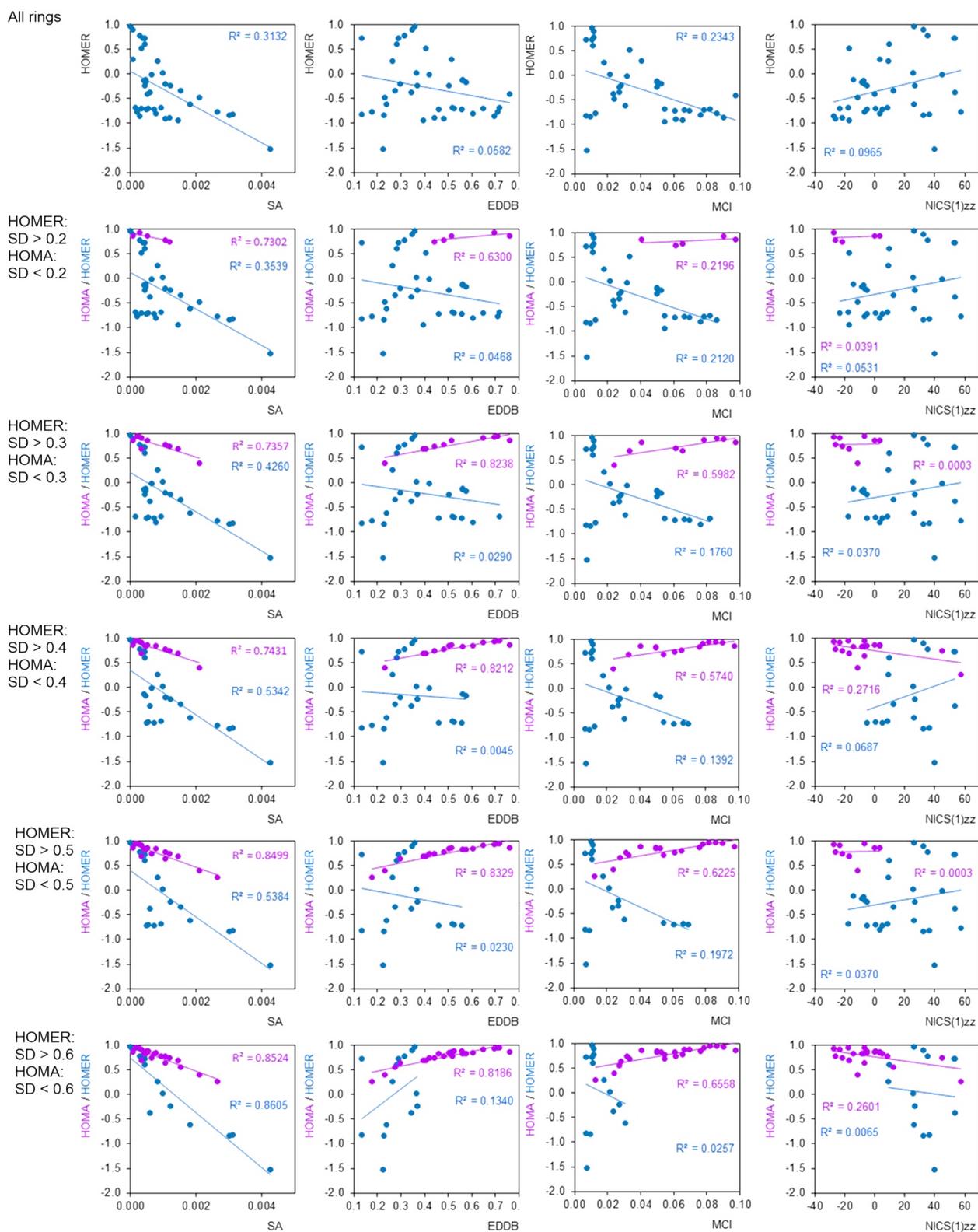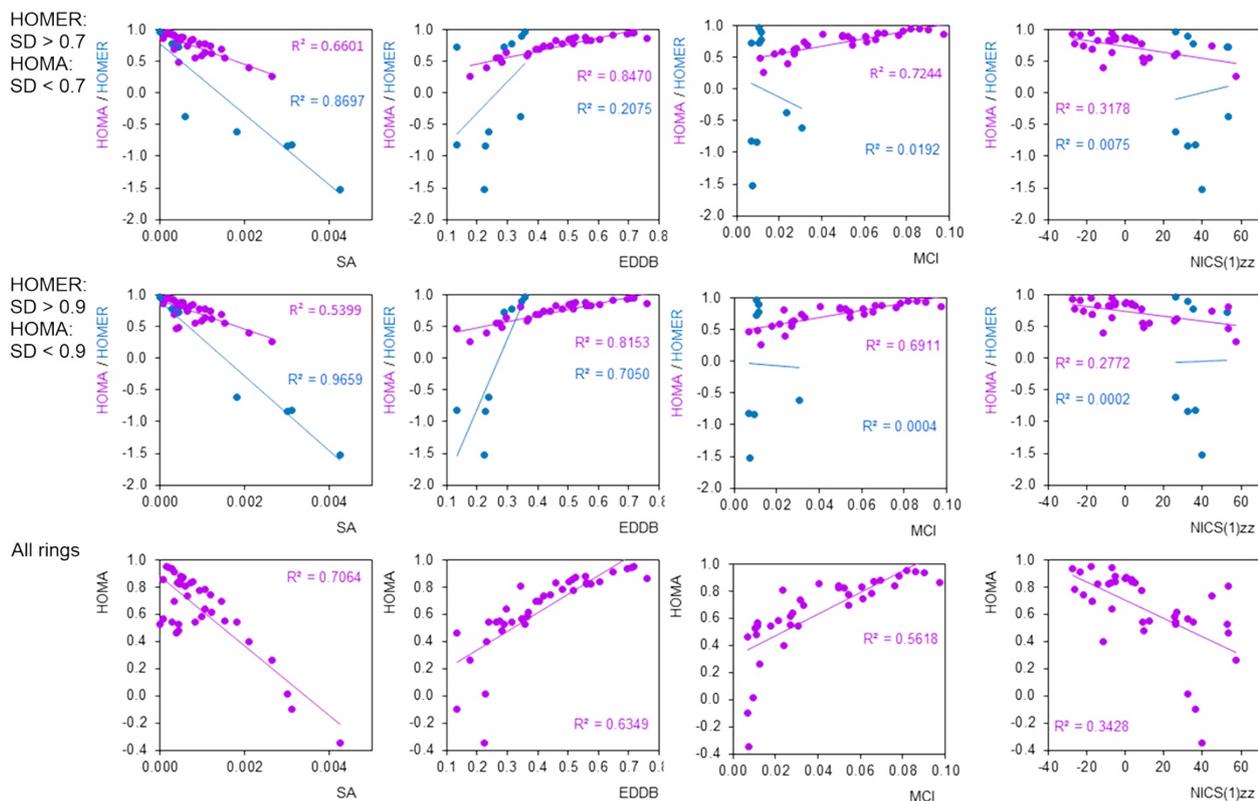
Figure S1. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for individual rings with different spin densities (SD) of polybenzenoid systems in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory.

All rings
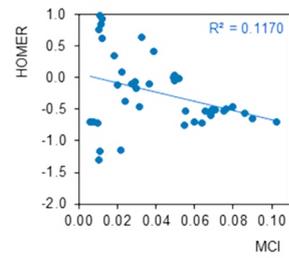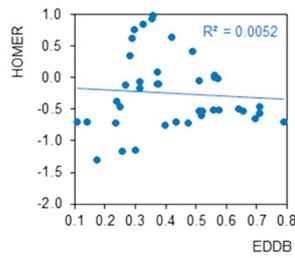
HOMER:
SD > 0.2
HOMA:
SD < 0.2

HOMER:
SD > 0.3
HOMA:
SD < 0.3
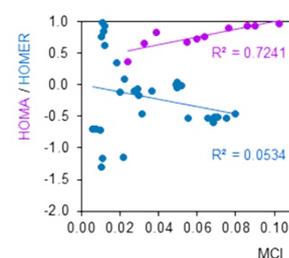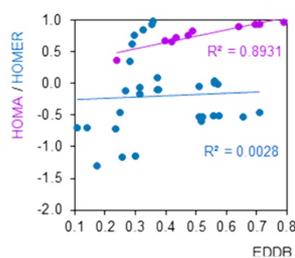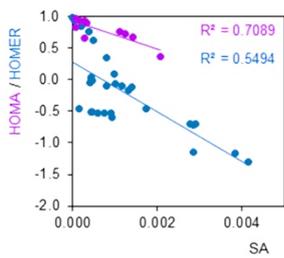
HOMER:
SD > 0.4
HOMA:
SD < 0.4
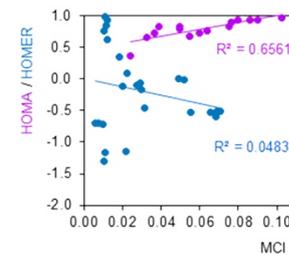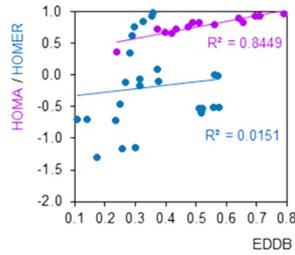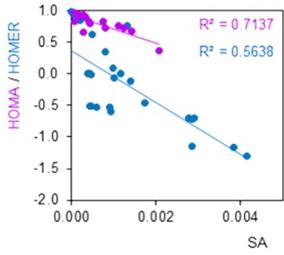
HOMER:
SD > 0.5
HOMA:
SD < 0.5

HOMER:
SD > 0.6
HOMA:
SD < 0.6

S17
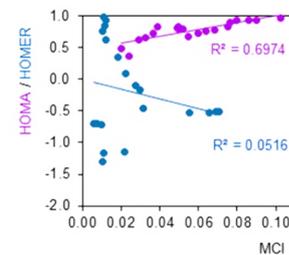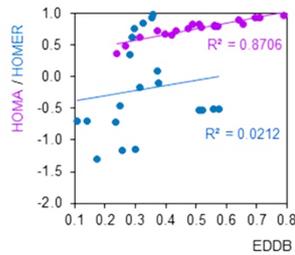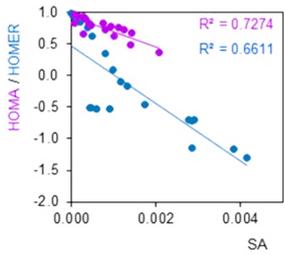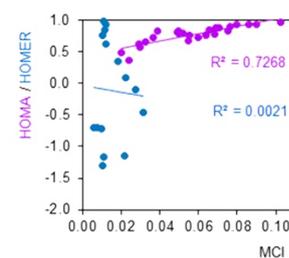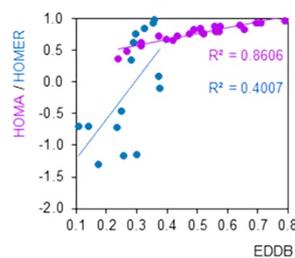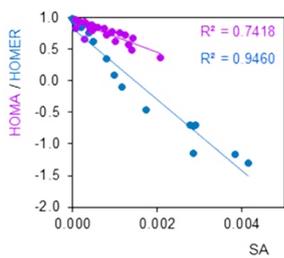
Figure S2. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and multicenter index (MCI) calculated for individual rings with different spin densities (SD) of polybenzenoid systems in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory.

Figure S3. Correlations between HOMA/HOMER and Shannon aromaticity (SA) and electron density of delocalized bonds per atom (EDDB) calculated for molecular perimeter of polybenzenoid systems in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory.

Figure S4. Correlations between HOMA/HOMER and Shannon aromaticity (SA) and electron density of delocalized bonds per atom (EDDB) calculated for molecular perimeter of polybenzenoid systems in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory.

Correlations for polycycles composed of benzene ring(s) and one cyclobutadiene ring (T_1)

Figure S5. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for cyclobutadiene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and one cyclobutadiene ring in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory.

Figure S6. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and multicenter index (MCI) calculated for cyclobutadiene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and one cyclobutadiene ring in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory.

All six-membered rings

HOMER:
SD > 0.2
HOMA:
SD < 0.2

HOMER:
SD > 0.3
HOMA:
SD < 0.3

HOMER:
SD > 0.4
HOMA:
SD < 0.4

HOMER:
SD > 0.7
HOMA:
SD < 0.7

HOMER:
SD > 0.8
HOMA:
SD < 0.8

Row 1 (All six-membered rings):
- $R^2 = 0.0098$ (SA)
- $R^2 = 0.1243$ (EDDB)
- $R^2 = 0.3304$ (MCI)
- $R^2 = 0.0519$ (NICS(1)zz)

Row 2 (SD 0.2):
- $R^2 = 0.5152$; $R^2 = 0.0304$ (SA)
- $R^2 = 0.5845$; $R^2 = 0.0722$ (EDDB)
- $R^2 = 0.9652$; $R^2 = 0.2914$ (MCI)
- $R^2 = 0.1036$; $R^2 = 0.0227$ (NICS(1)zz)

Row 3 (SD 0.3):
- $R^2 = 0.8137$; $R^2 = 0.0611$ (SA)
- $R^2 = 0.9006$; $R^2 = 0.0642$ (EDDB)
- $R^2 = 0.9753$; $R^2 = 0.3571$ (MCI)
- $R^2 = 0.4816$; $R^2 = 0.0314$ (NICS(1)zz)

Row 4 (SD 0.4):
- $R^2 = 0.9049$; $R^2 = 0.0266$ (SA)
- $R^2 = 0.8474$; $R^2 = 0.0160$ (EDDB)
- $R^2 = 0.7964$; $R^2 = 0.2554$ (MCI)
- $R^2 = 0.2853$; $R^2 = 0.0395$ (NICS(1)zz)

Row 5 (SD 0.7):
- $R^2 = 0.8198$; $R^2 = 0.0111$ (SA)
- $R^2 = 0.8035$; $R^2 = 0.0002$ (EDDB)
- $R^2 = 0.8136$; $R^2 = 0.4013$ (MCI)
- $R^2 = 0.2252$; $R^2 = 0.1034$ (NICS(1)zz)

Row 6 (SD 0.8):
- $R^2 = 0.7951$; $R^2 = 0.0096$ (SA)
- $R^2 = 0.8079$; $R^2 = 0.0045$ (EDDB)
- $R^2 = 0.8080$; $R^2 = 0.3901$ (MCI)
- $R^2 = 0.1968$; $R^2 = 0.0867$ (NICS(1)zz)

Axis labels: HOMER, HOMA / HOMER (y-axes); SA, EDDB, MCI, NICS(1)zz (x-axes)

S22

Figure S7. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for benzene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and one cyclobutadiene ring in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory.

S23

All six-membered rings

HOMER: SD > 0.2 HOMA: SD < 0.2

HOMER: SD > 0.3 HOMA: SD < 0.3

HOMER: SD > 0.4 HOMA: SD < 0.4

HOMER: SD > 0.6 HOMA: SD < 0.6

HOMER: SD > 0.8 HOMA: SD < 0.8

S24
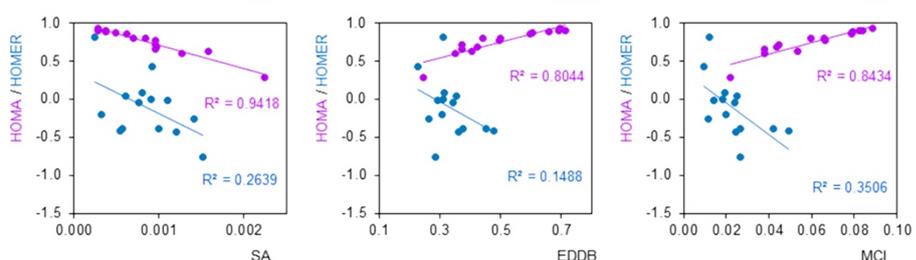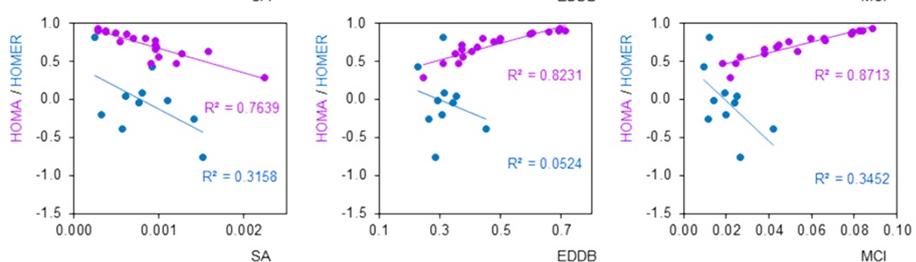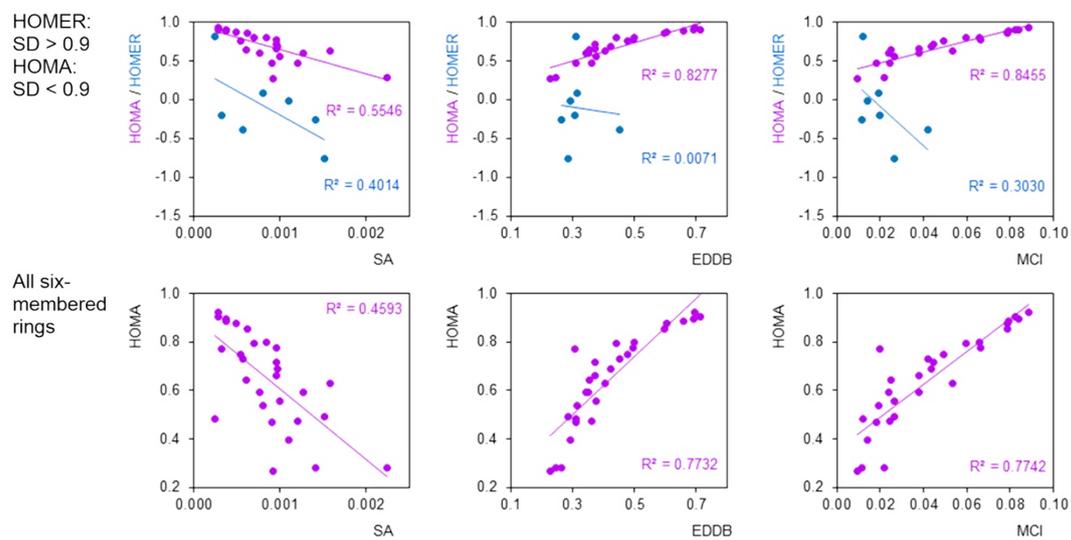
Figure S8. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and multicenter index (MCI) calculated for benzene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and one cyclobutadiene ring in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory.
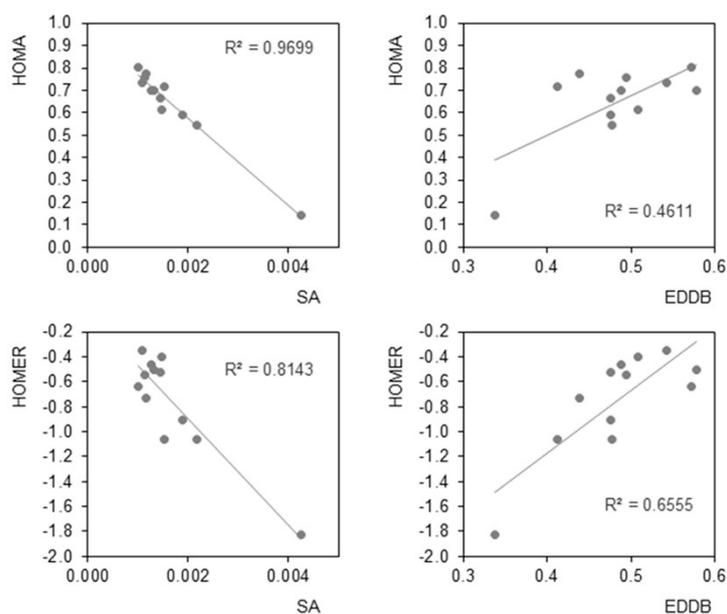
Figure S9. Correlations between HOMA/HOMER and Shannon aromaticity (SA) and electron density of delocalized bonds per atom (EDDB) calculated for molecular perimeter of polycycles composed of benzene ring(s) and one cyclobutadiene ring in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory.
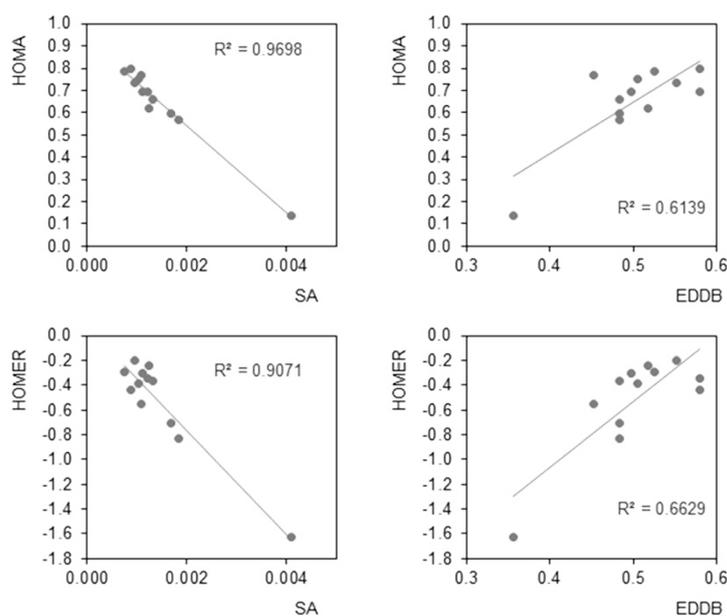
Figure S10. Correlations between HOMA/HOMER and Shannon aromaticity (SA) and electron density of delocalized bonds per atom (EDDB) calculated for molecular perimeter of polycycles composed of benzene ring(s) and one cyclobutadiene ring in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory.

Correlations for polycycles composed of benzene ring(s) and one cyclooctatetraene ring (T$_1$)
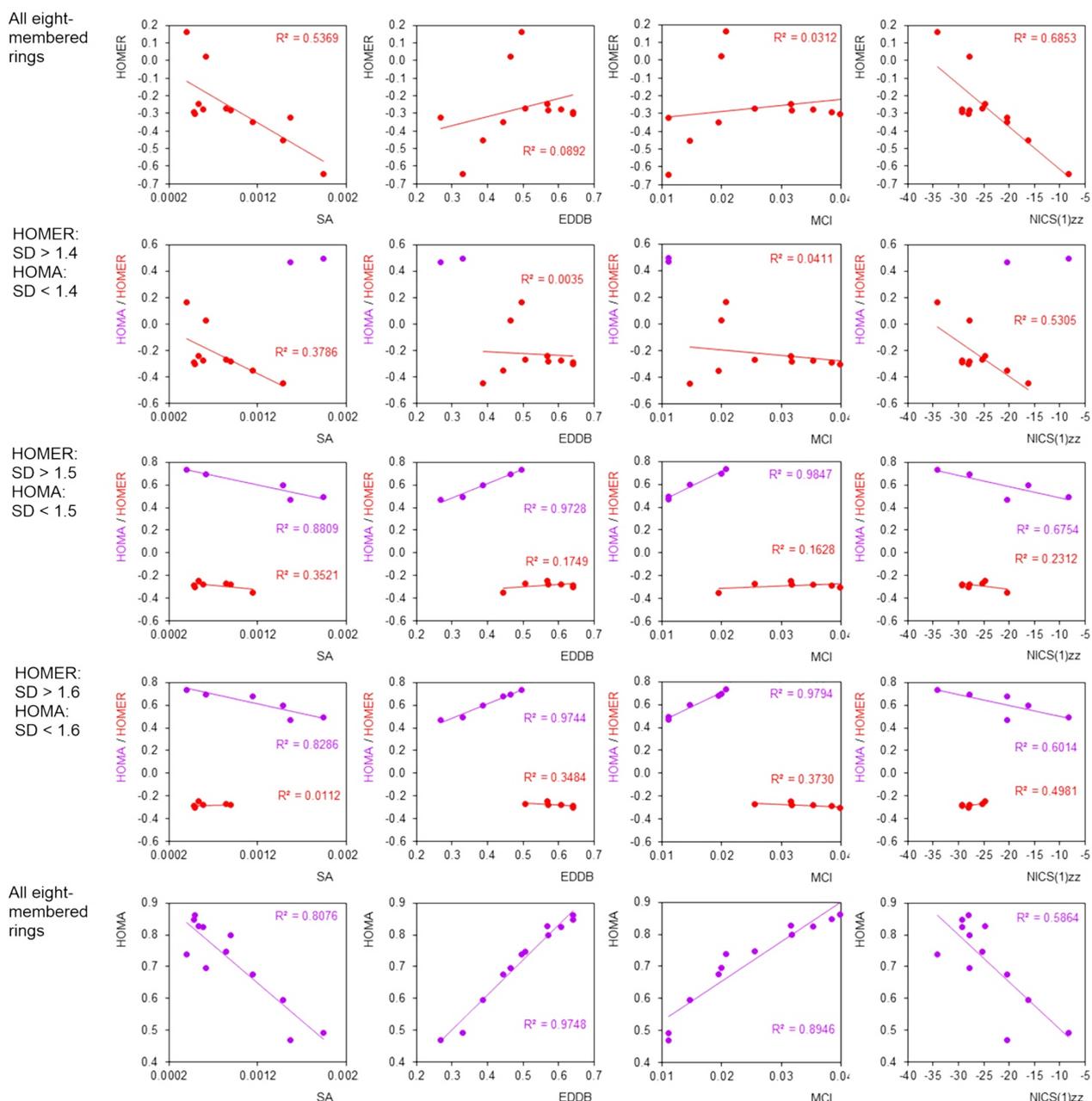
Figure S11. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for cyclooctatetraene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and one cyclooctatetraene ring in their T$_1$ state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory.
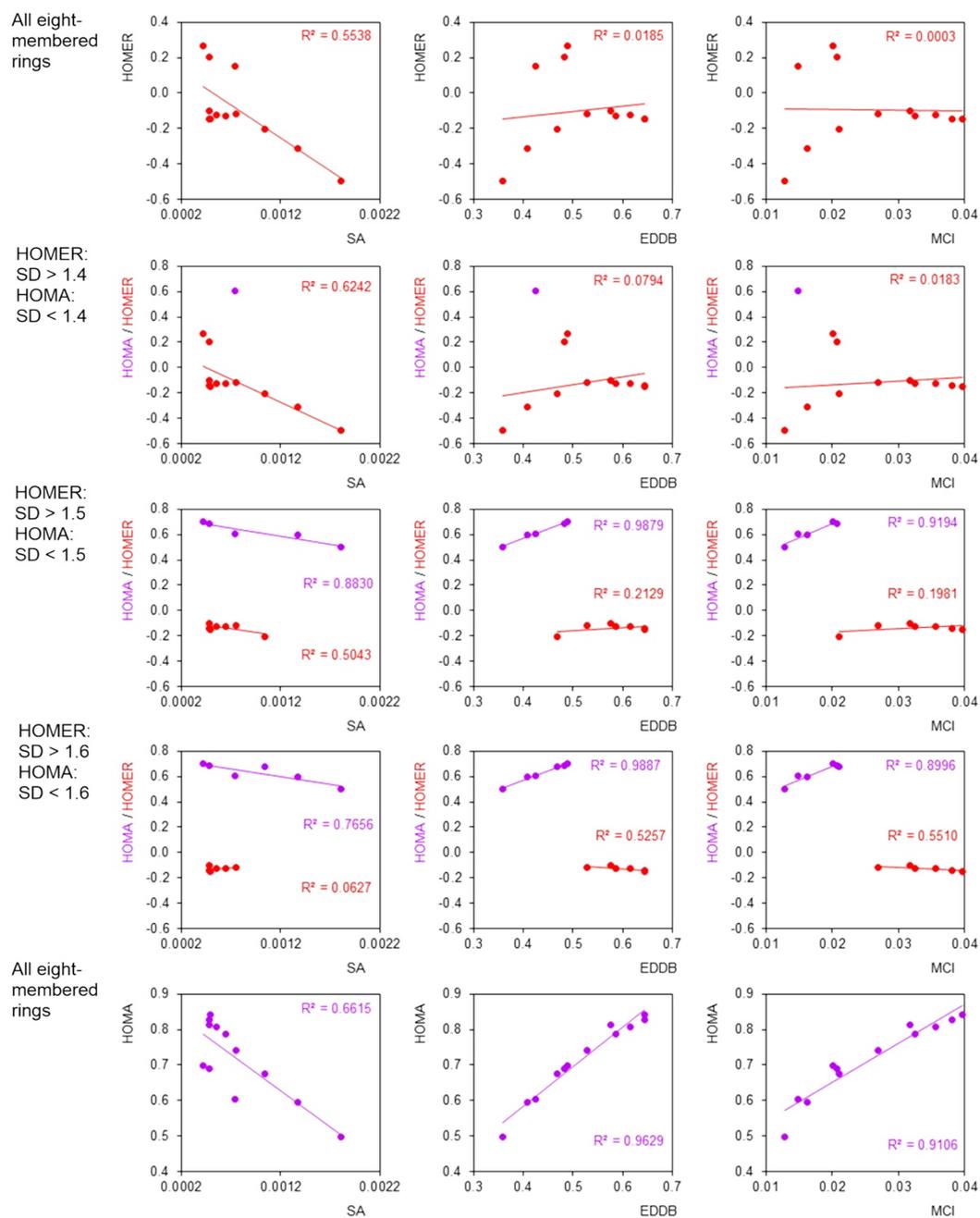
Figure S12. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and multicenter index (MCI) calculated for cyclooctatetraene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and one cyclooctatetraene ring in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory.
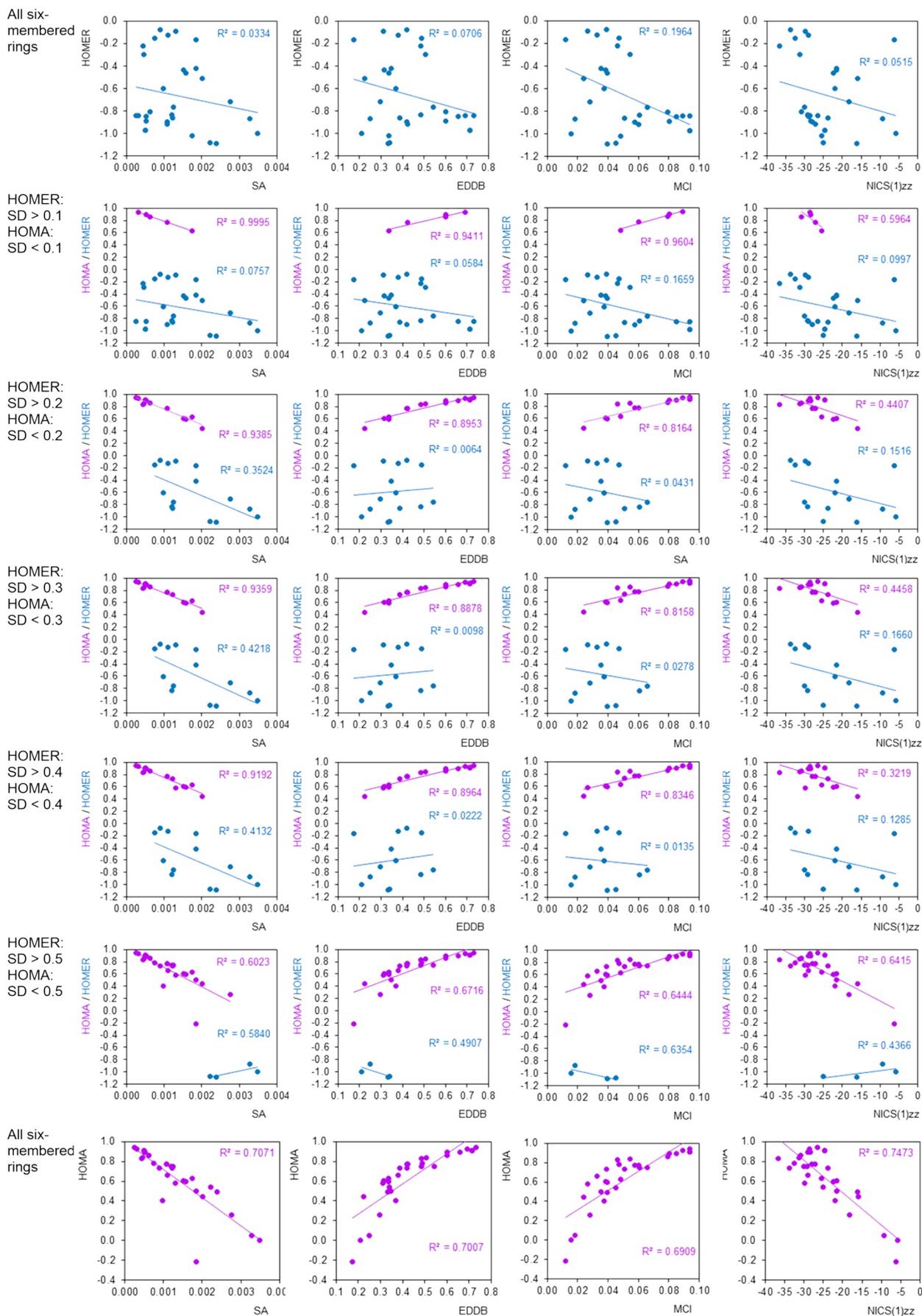
Figure S13. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for benzene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and one cyclooctatetraene ring in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory.
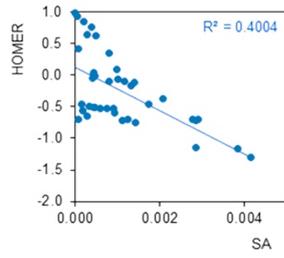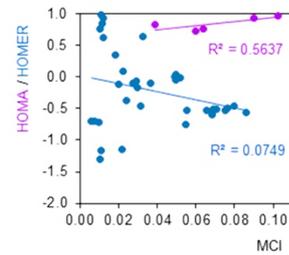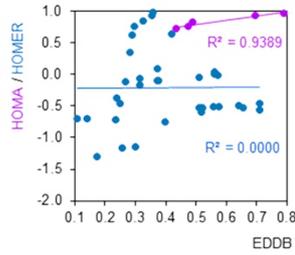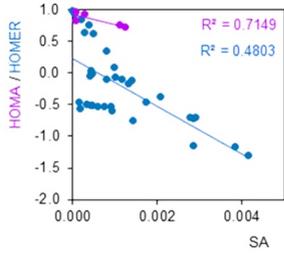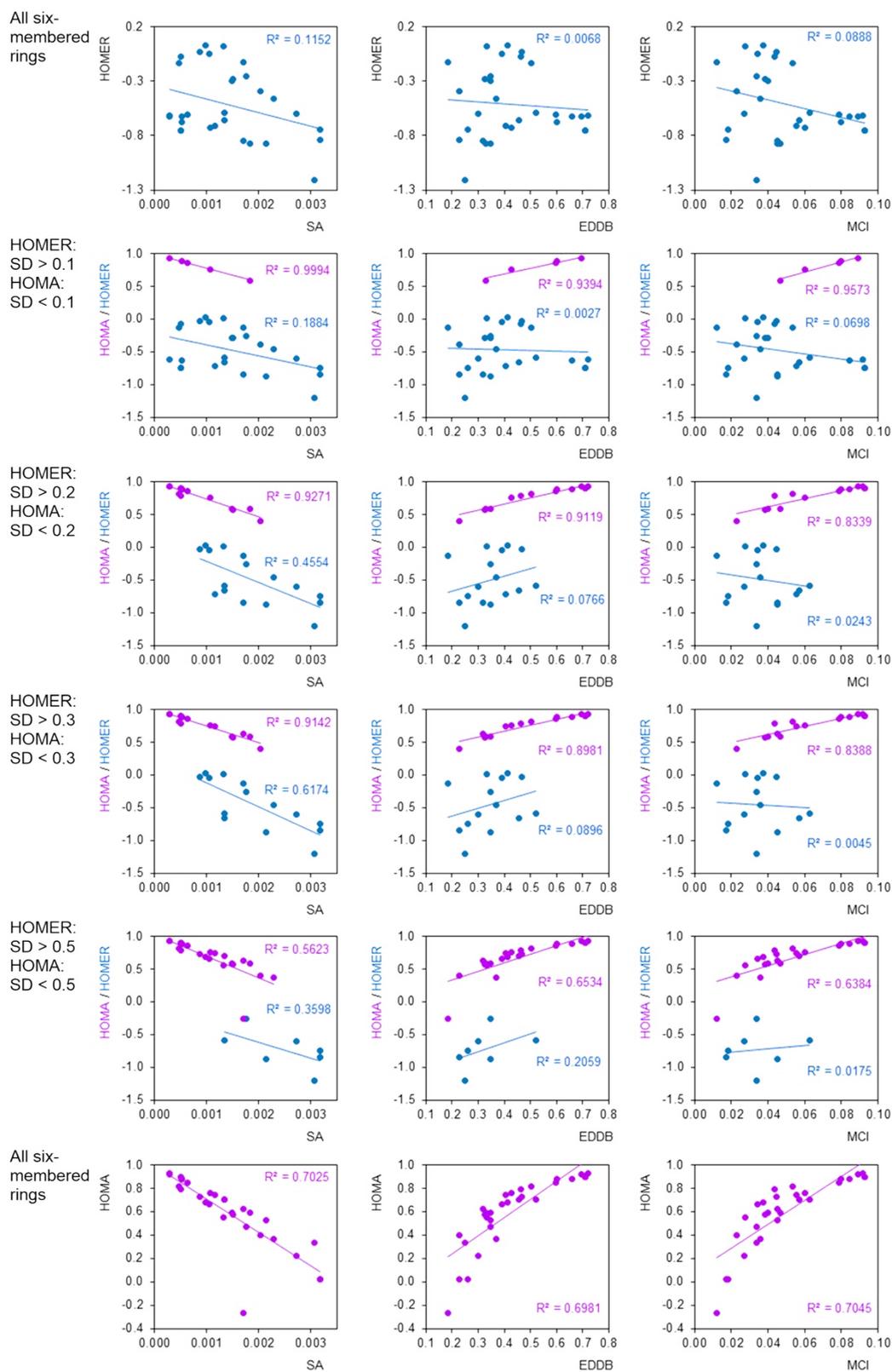
Figure S14. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and multicenter index (MCI) calculated for benzene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and one cyclooctatetraene ring in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory.
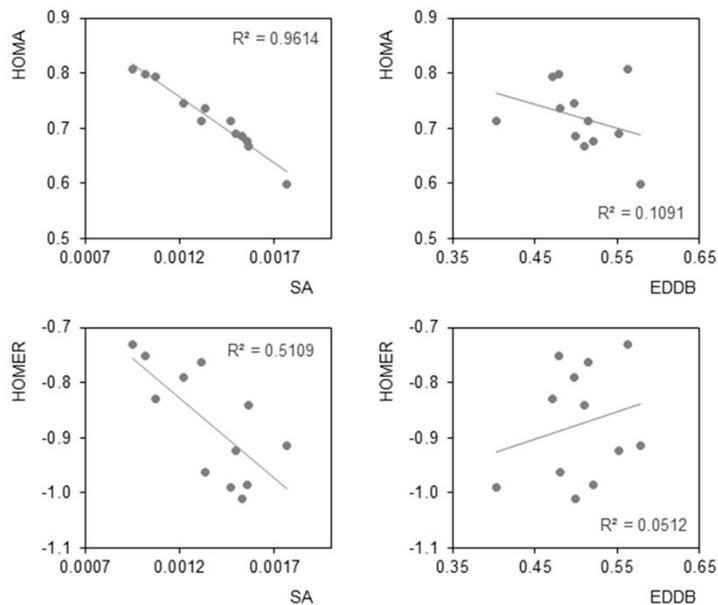
Figure S15. Correlations between HOMA/HOMER and Shannon aromaticity (SA) and electron density of delocalized bonds per atom (EDDB) calculated for molecular perimeter of polycycles composed of benzene ring(s) and one cyclooctatetraene ring in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory.
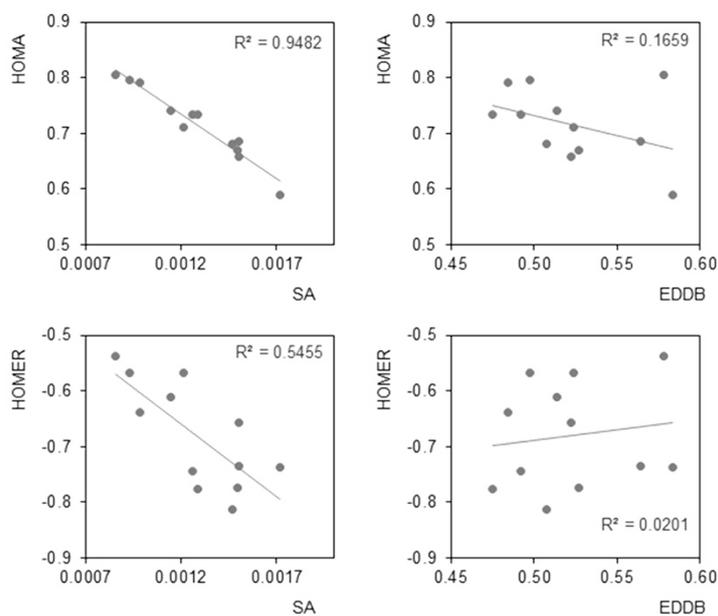
Figure S16. Correlations between HOMA/HOMER and Shannon aromaticity (SA) and electron density of delocalized bonds per atom (EDDB) calculated for molecular perimeter of polycycles composed of benzene ring(s) and one cyclooctatetraene ring in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory.

Correlations for polycycles composed of benzene ring(s) and pentalene core (T_1)
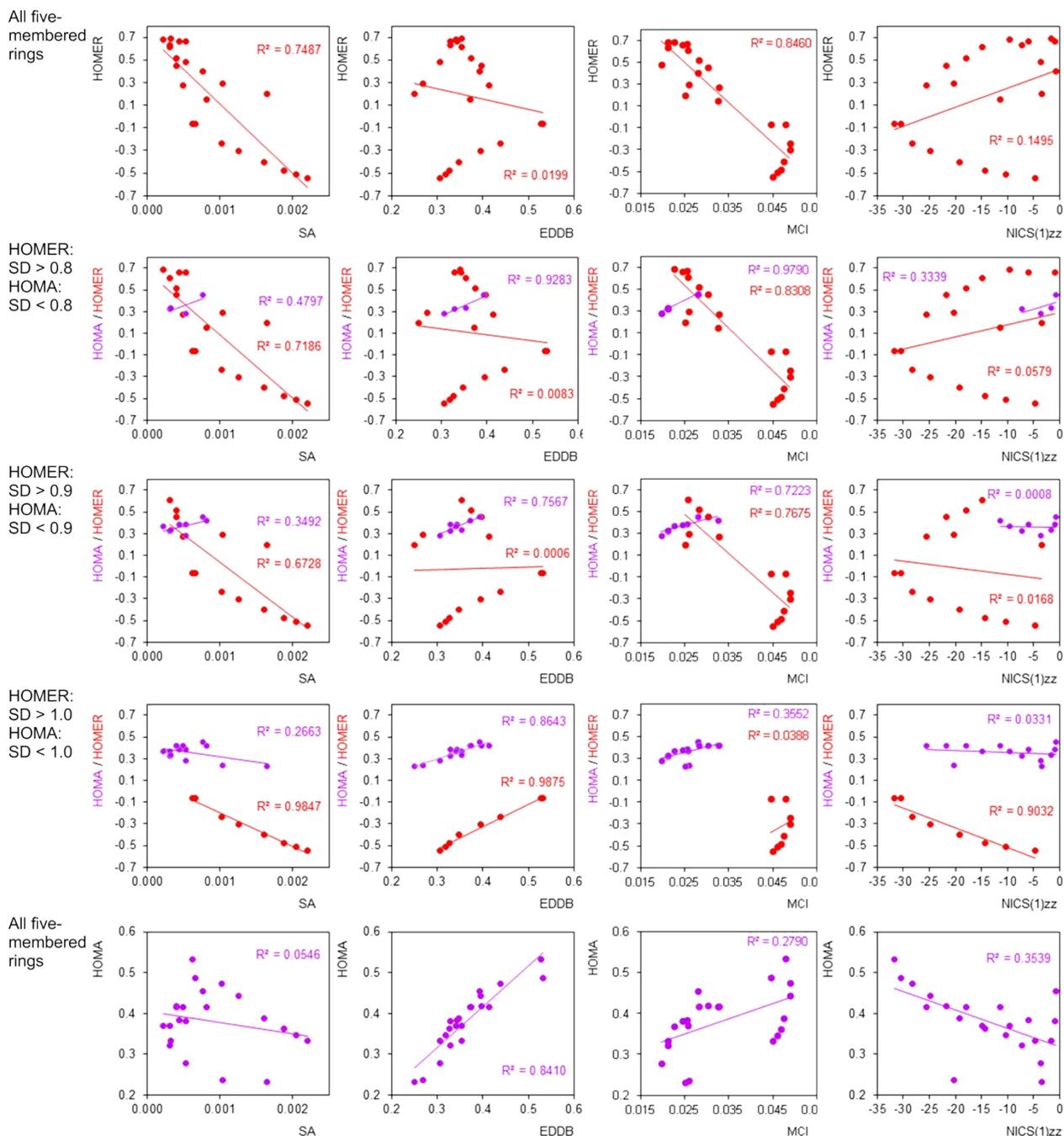
Figure S17. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for five-membered rings with different spin densities (SD) of polycycles composed of benzene ring(s) and pentalene core in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory. Pentalene is included in correlations.
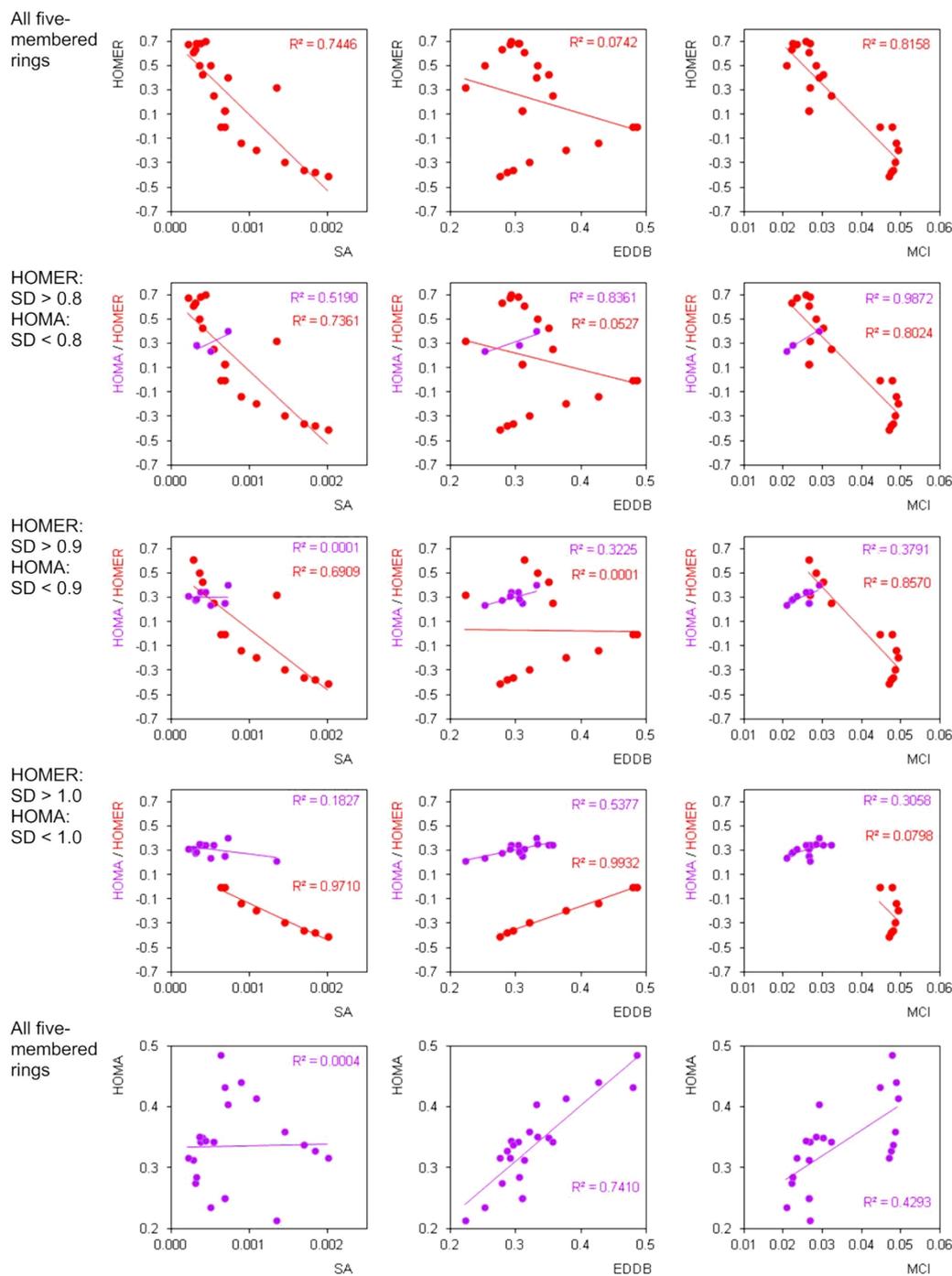
Figure S18. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and multicenter index (MCI) and calculated for five-membered rings with different spin densities (SD) of polycycles composed of benzene ring(s) and pentalene core in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory. Pentalene is included in correlations.
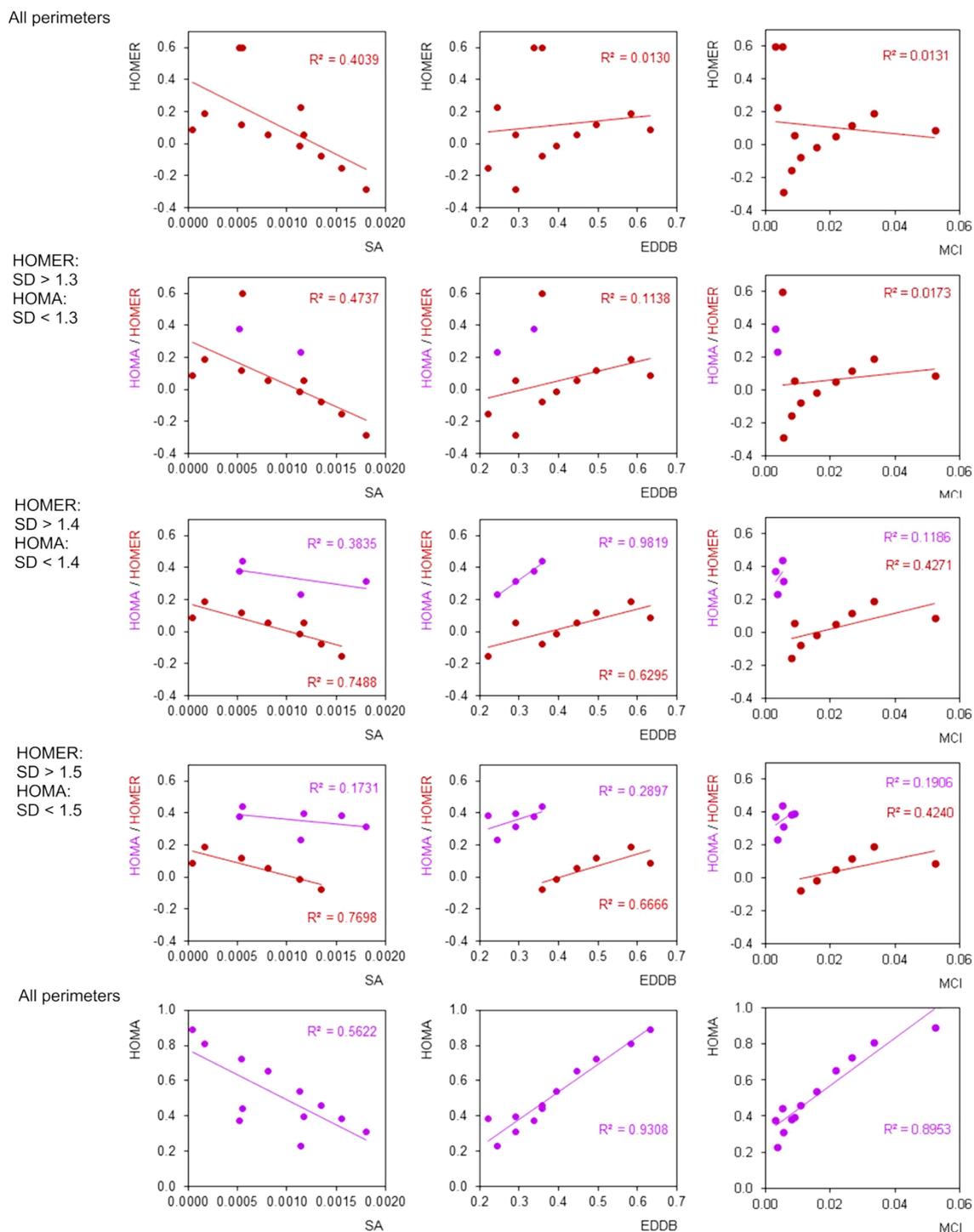
Figure S19. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and multicenter index (MCI) calculated for perimeter of pentalene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and pentalene core in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory. Pentalene is included in correlations.
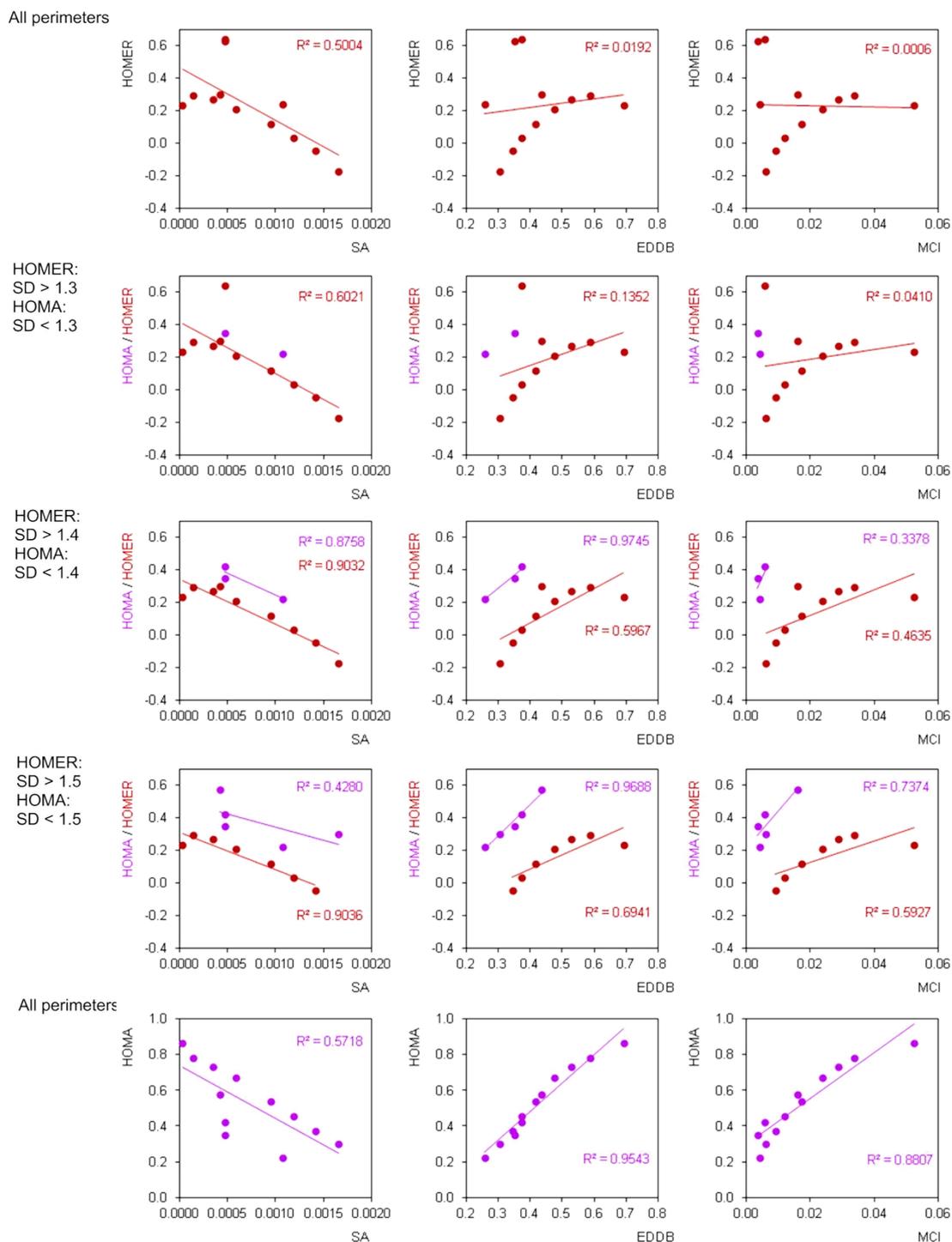
Figure S20. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and multicenter index (MCI) calculated for perimeter of pentalene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and pentalene core in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory. Pentalene is included in correlations.
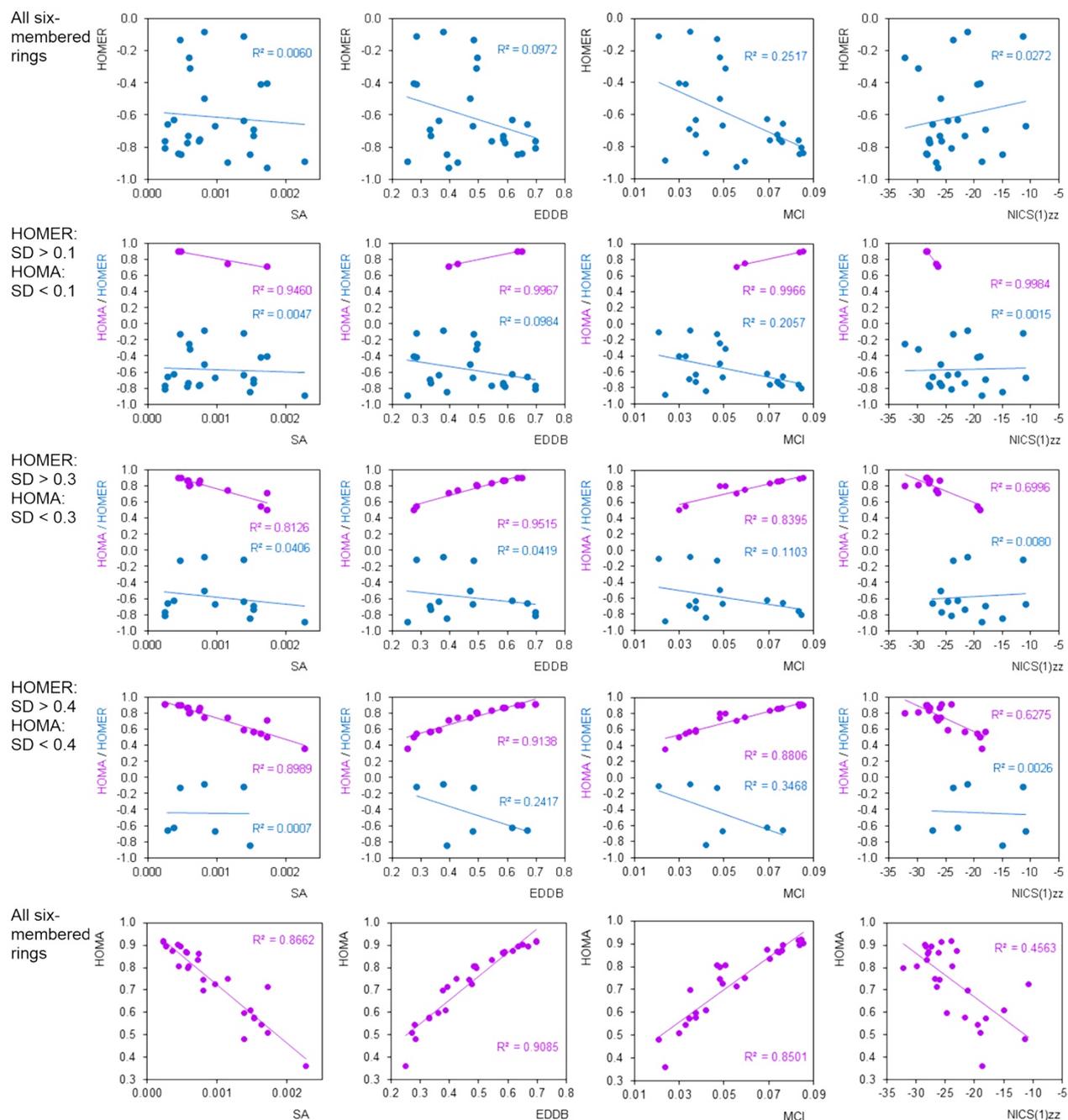
Figure S21. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for benzene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and pentalene core in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory.

Figure S22. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for benzene subunits with different spin densities (SD) of polycycles composed of benzene ring(s) and pentalene core in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory.
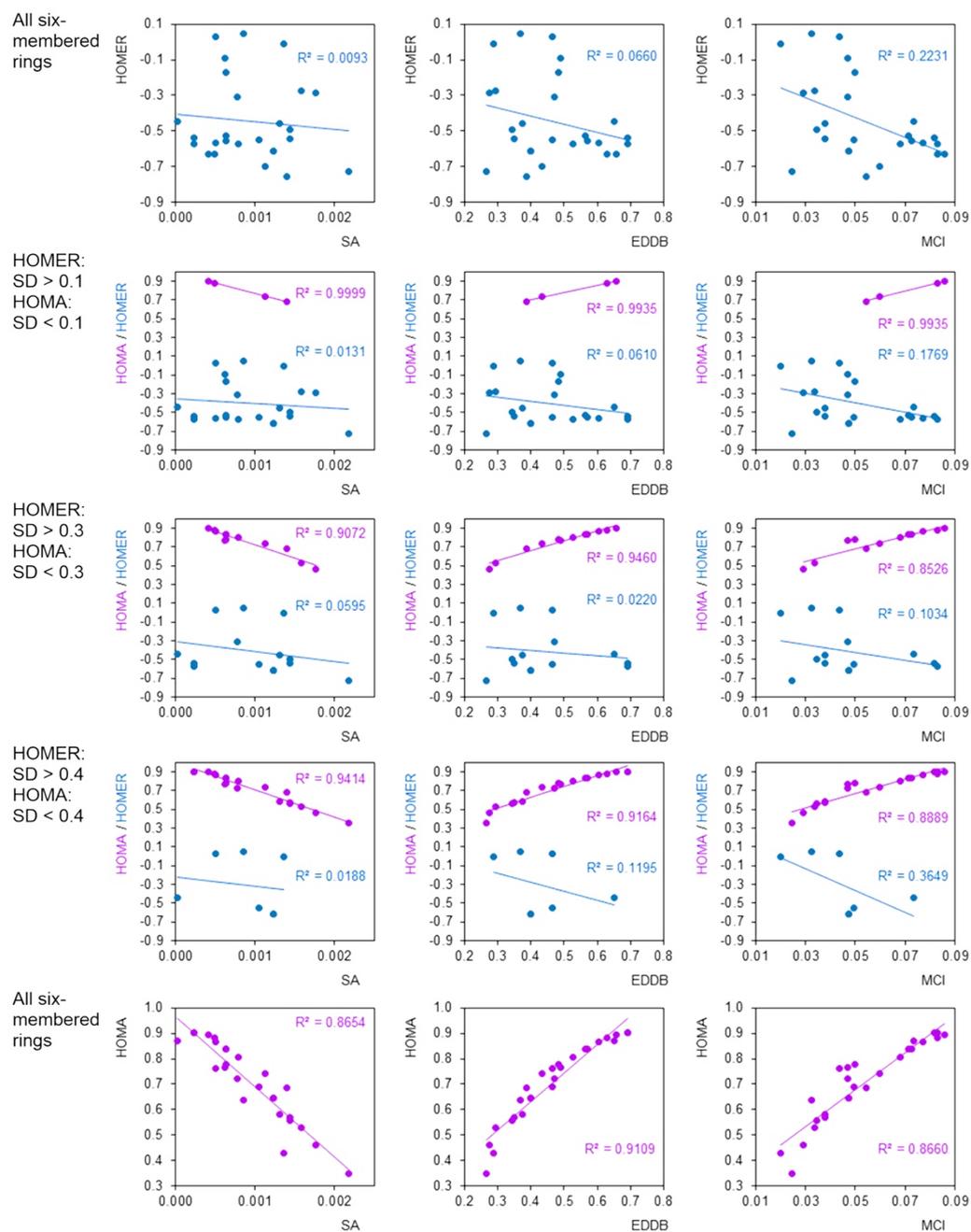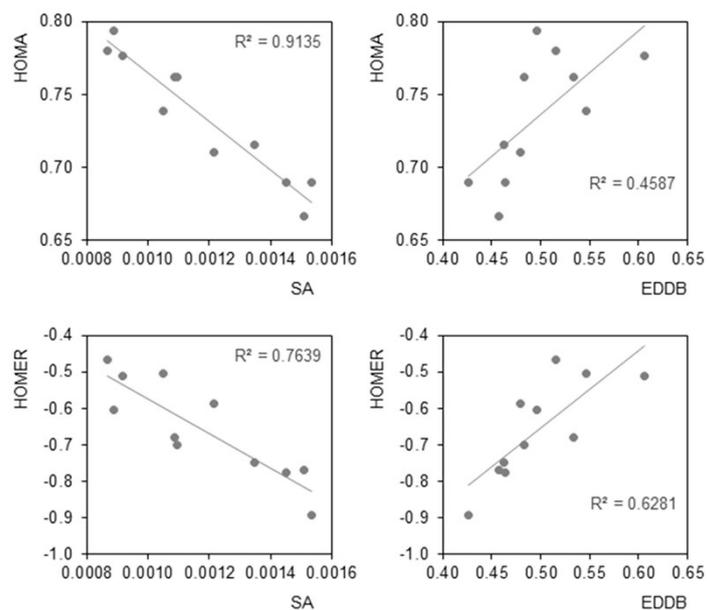
Figure S23. Correlations between HOMA/HOMER and Shannon aromaticity (SA) and electron density of delocalized bonds per atom (EDDB) calculated for molecular perimeter of polycycles composed of benzene ring(s) and pentalene core in their T_1 state. Calculations were performed at the UCAM-B3LYP/6-311+G(d,p) level of theory.
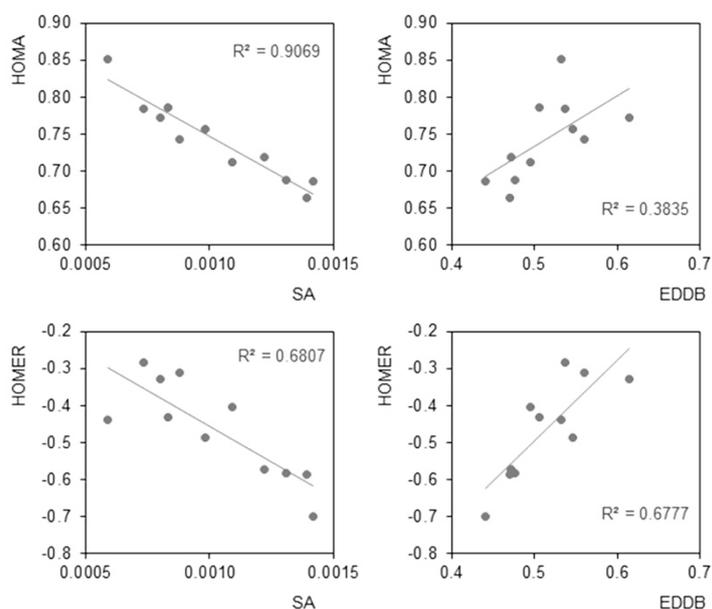
Figure S24. Correlations between HOMA/HOMER and Shannon aromaticity (SA) and electron density of delocalized bonds per atom (EDDB) calculated for molecular perimeter of polycycles composed of benzene ring(s) and pentalene core in their T_1 state. Calculations were performed at the UM06-2X/6-311+G(d,p) level of theory.

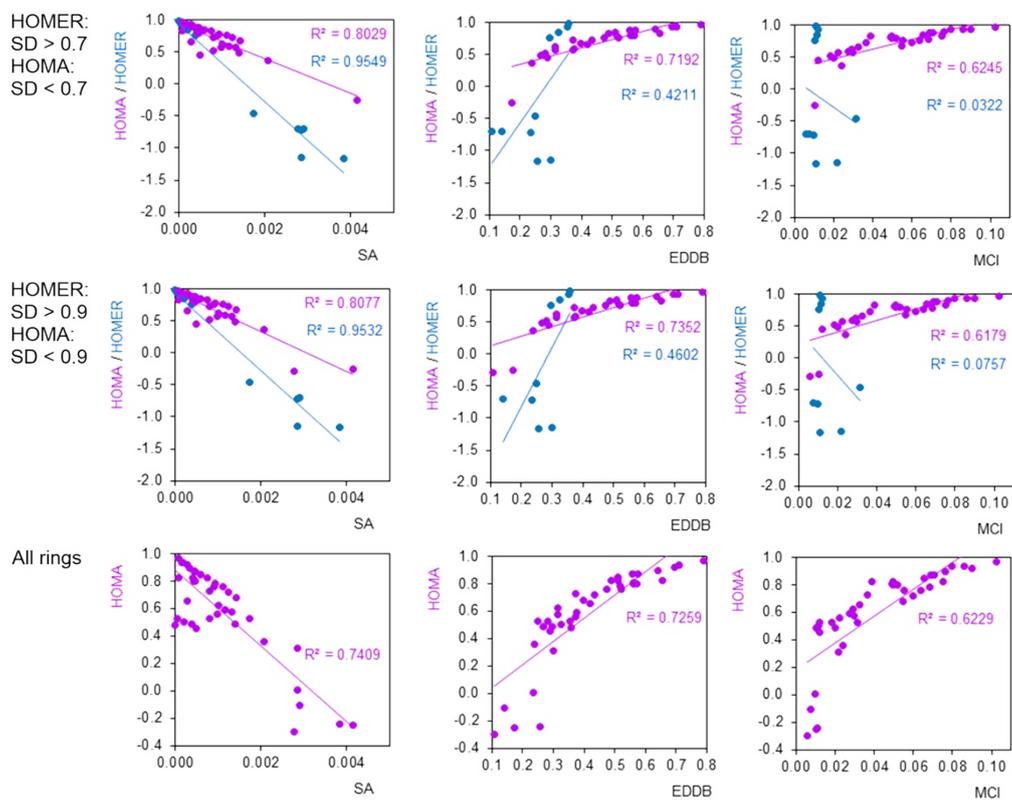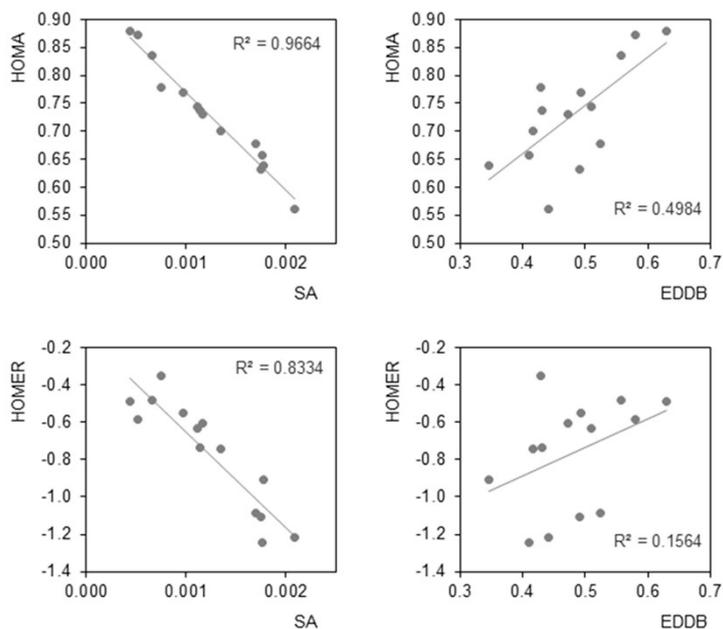# Correlations for polybenzenoid compounds (S$_0$)
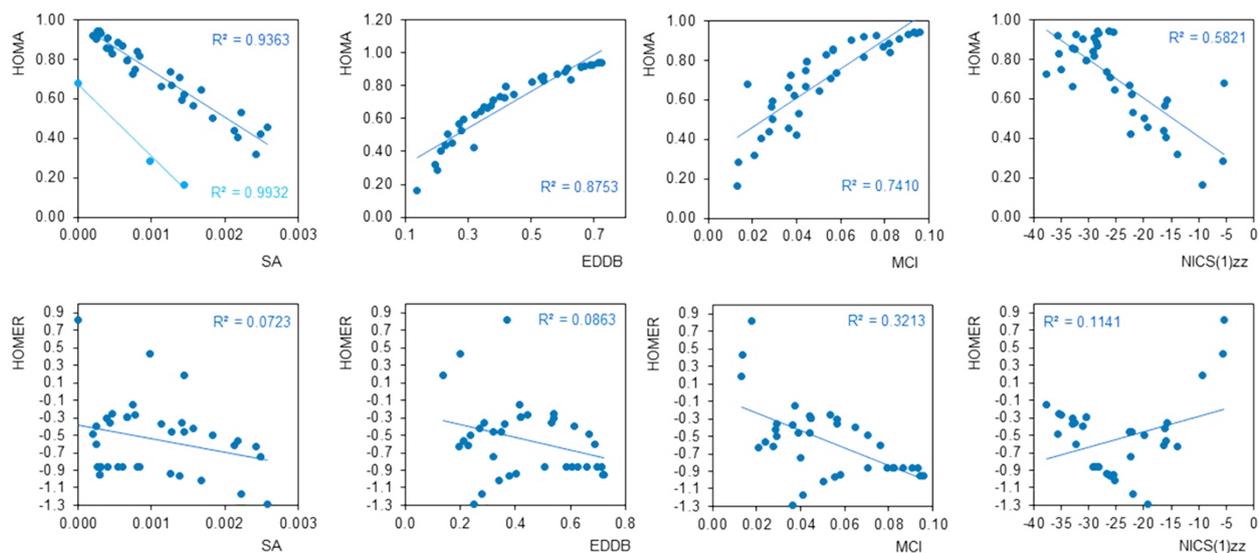
Figure S25. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for individual rings of polybenzenoid systems in their S$_0$ state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. Light blue corresponds to the central rings of triphenylene, benzo[e]pyrene and coronene.
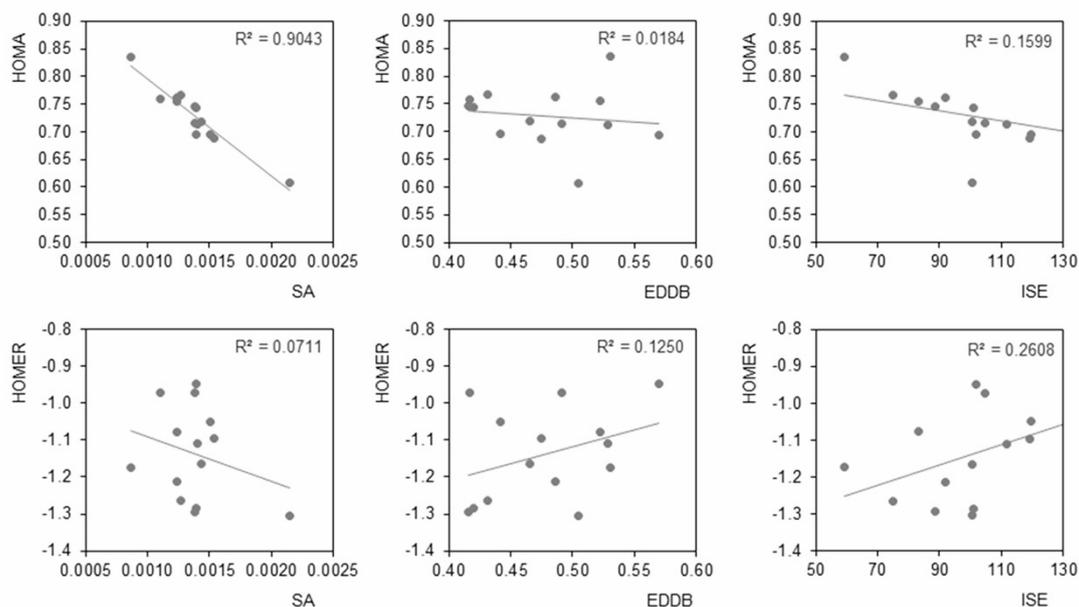
Figure S26. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and isomerization stabilization energy (ISE) calculated for molecular perimeter of polybenzenoid systems in their S$_0$ state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. ISE schemes are shown in Figure S37.
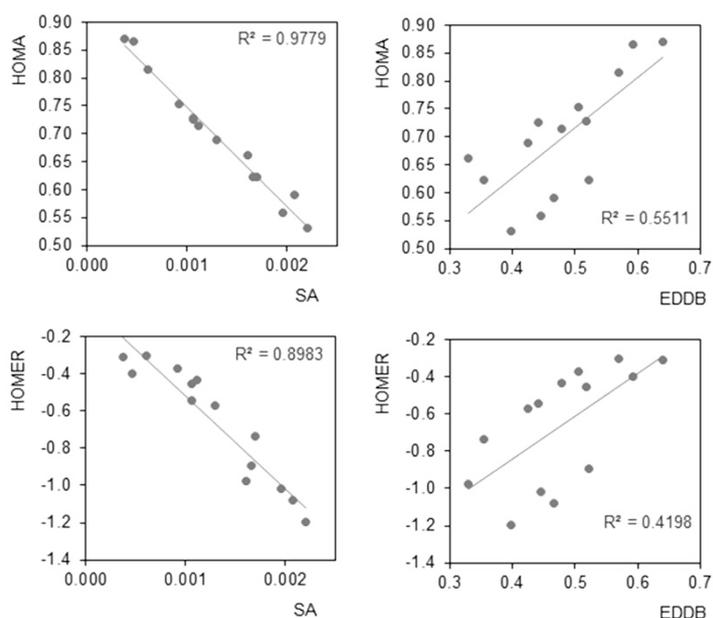
Correlations for polycycles composed of benzene ring(s) and one cyclobutadiene ring (S_0)
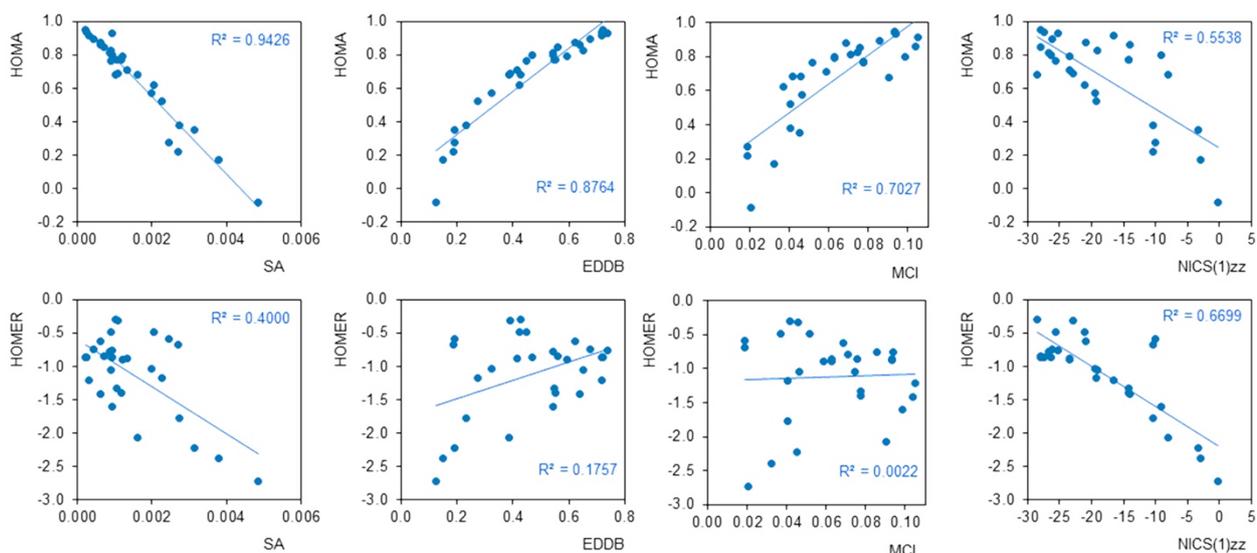
Figure S27. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for six-membered rings of polycycles composed of benzene ring(s) and one cyclobutadiene ring in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory.
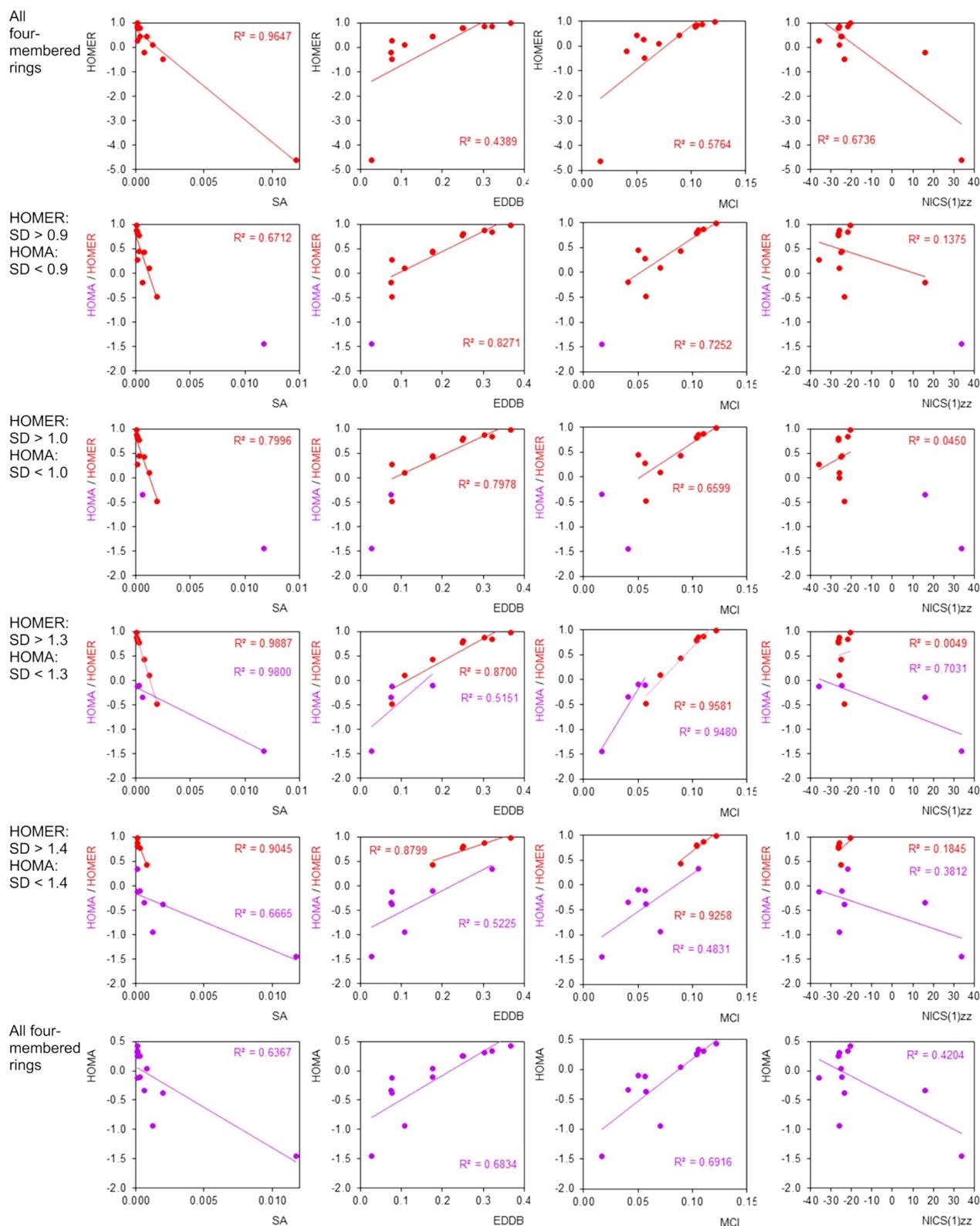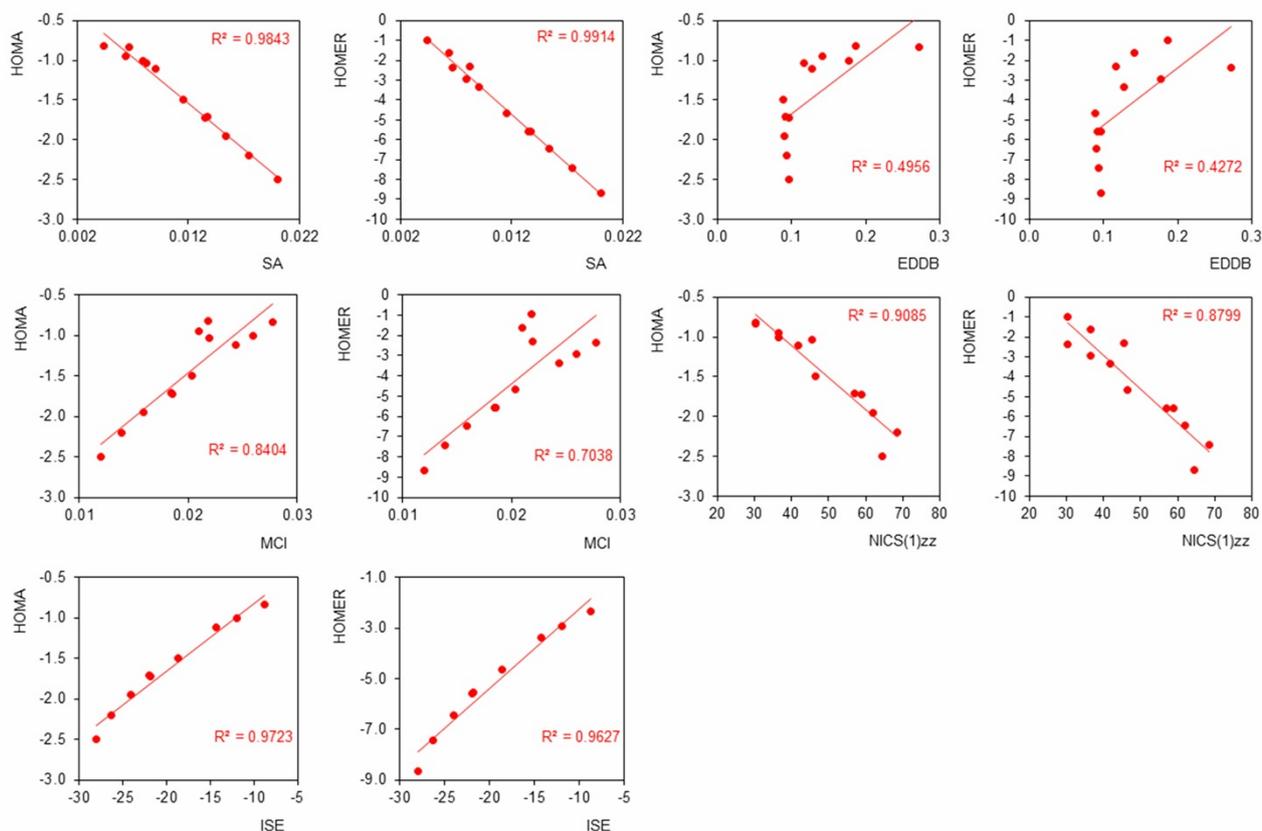

Figure S28. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI), NICS(1)$_{zz}$ and isomerization stabilization energy (ISE) calculated for four-membered rings of polycycles composed of benzene ring(s) and one cyclobutadiene ring in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. The systems involved in correlations with ISE are shown in Figure S38.
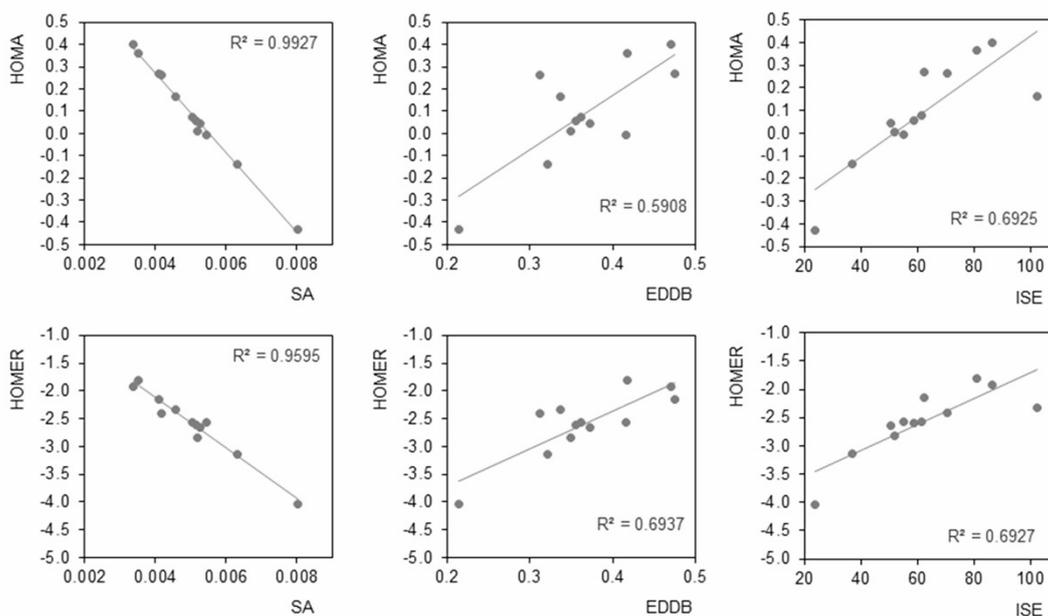
Figure S29. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and isomerization stabilization energy (ISE) calculated for molecular perimeter of polycycles composed of benzene ring(s) and one cyclobutadiene ring in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. ISE schemes are shown in Figure S39.
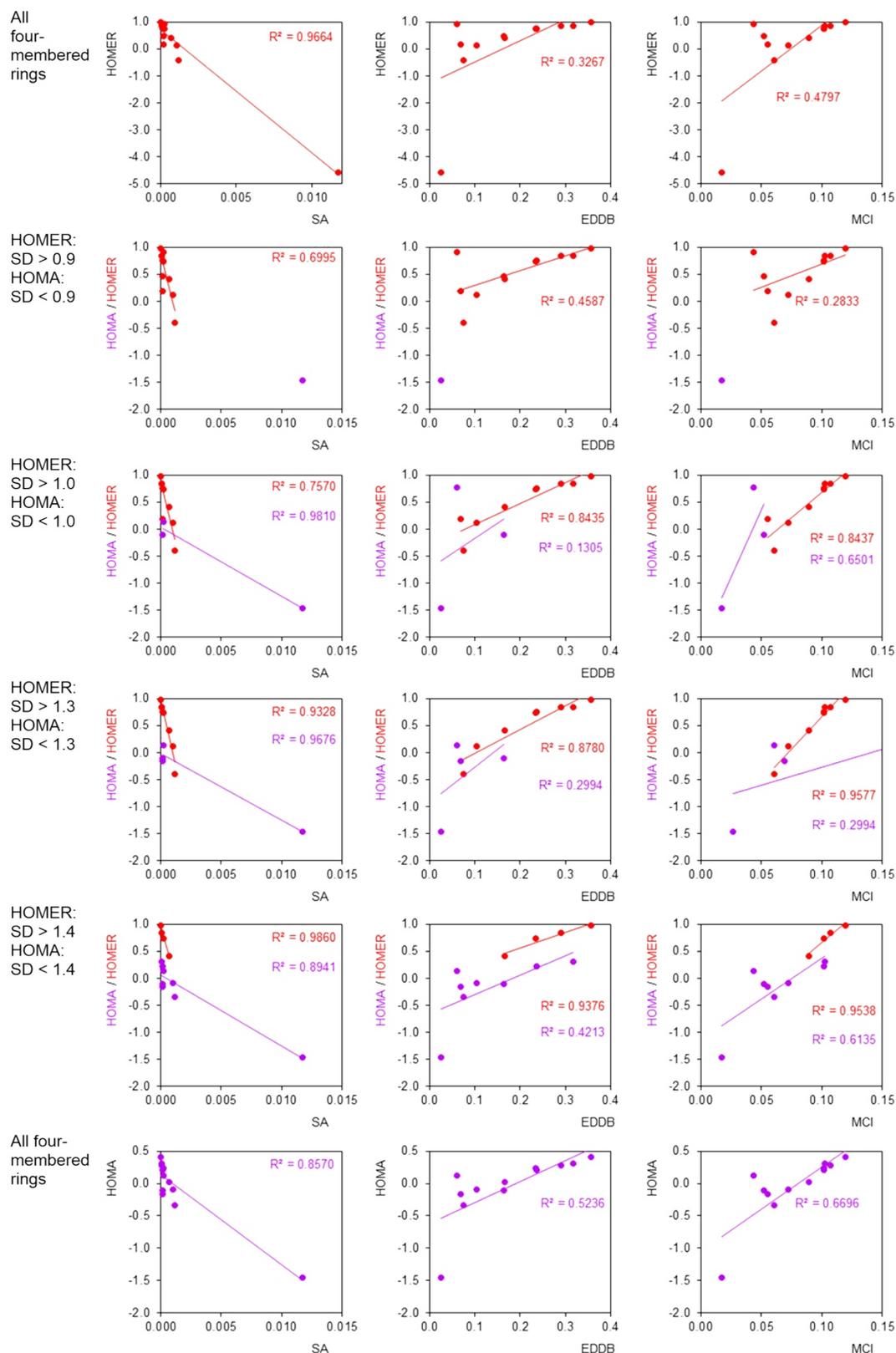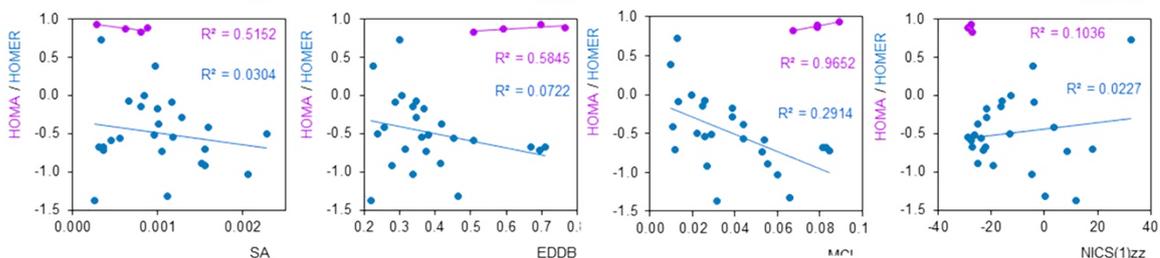
Correlations for polycycles composed of benzene ring(s) and one cyclooctatetraene ring (S_0)
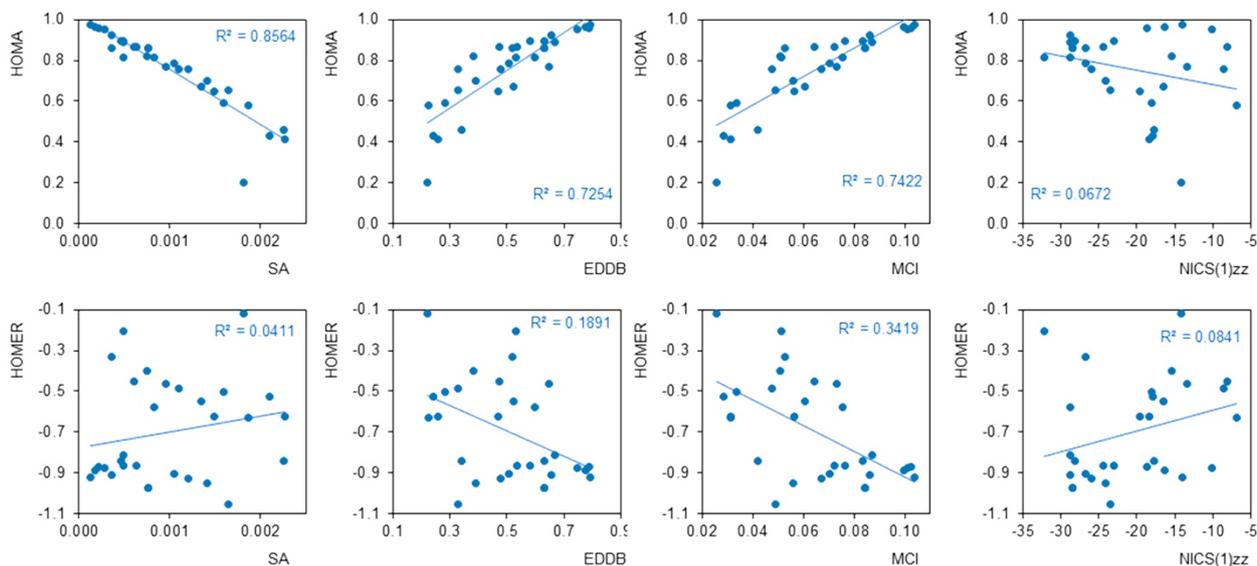
Figure S30. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for benzene subunits of polycycles composed of benzene ring(s) and one cyclooctatetraene ring in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory.
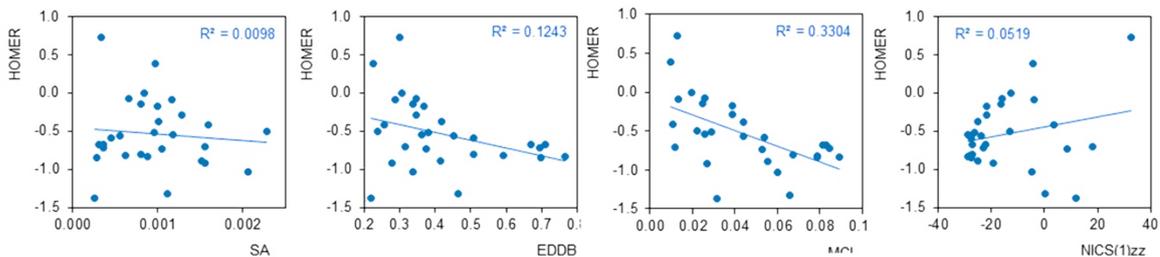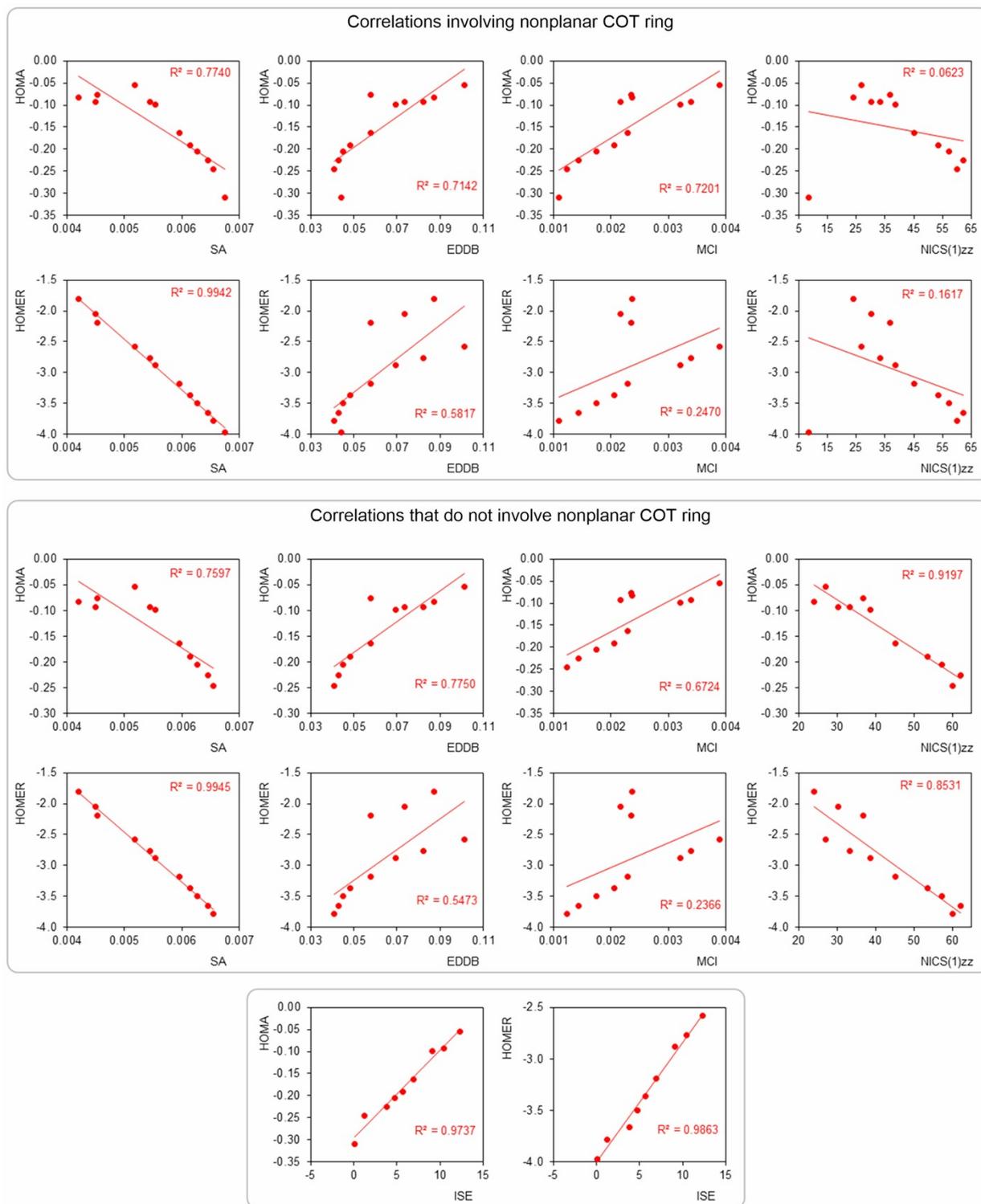
Figure S31. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI), NICS(1)$_{zz}$ and isomerization stabilization energy (ISE) calculated for cyclooctatetraene subunits of polycycles composed of benzene ring(s) and one cycloocta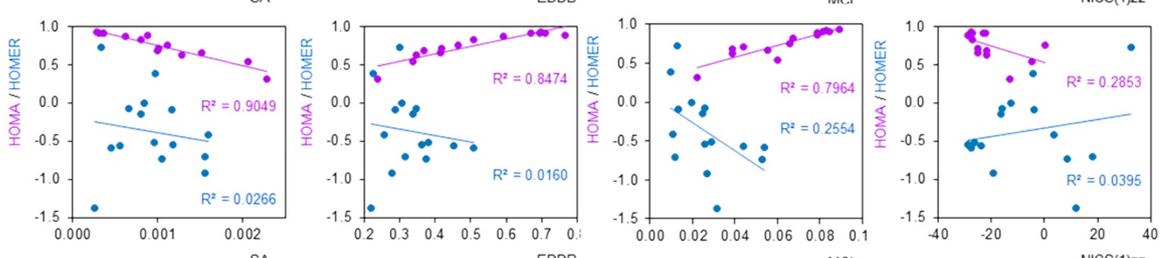tetraene ring in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. The systems involved in correlations with ISE are shown in Figure S40.
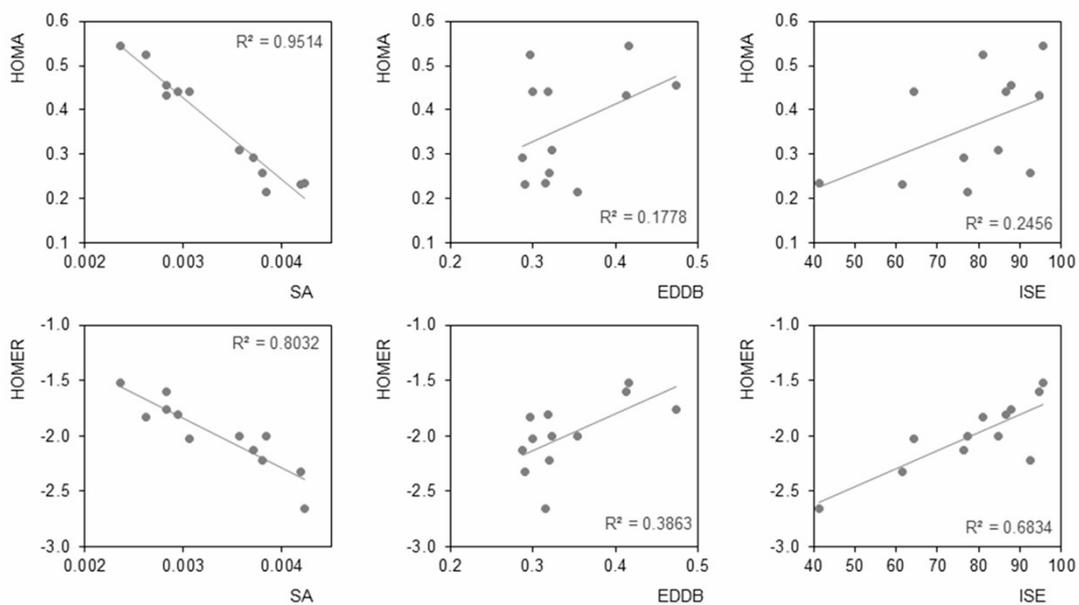
Figure S32. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and isomerization stabilization energy (ISE) calculated for molecular perimeter of polycycles composed of benzene ring(s) and one cyclooctatetraene ring in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. ISE schemes are shown in Figure S41.

Correlations for polycycles composed of benzene ring(s) and pentalene core (S_0)
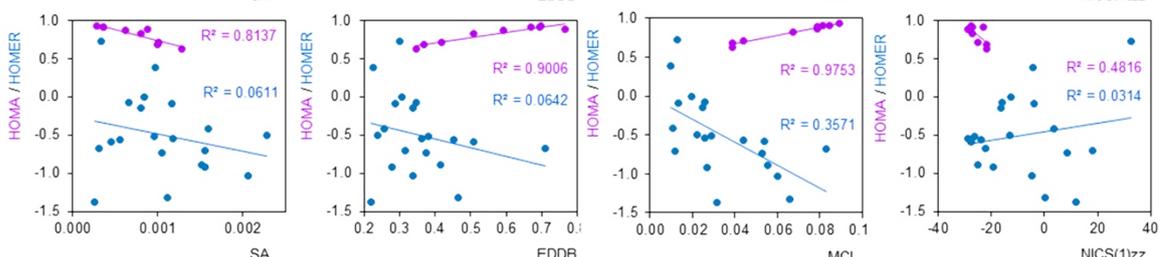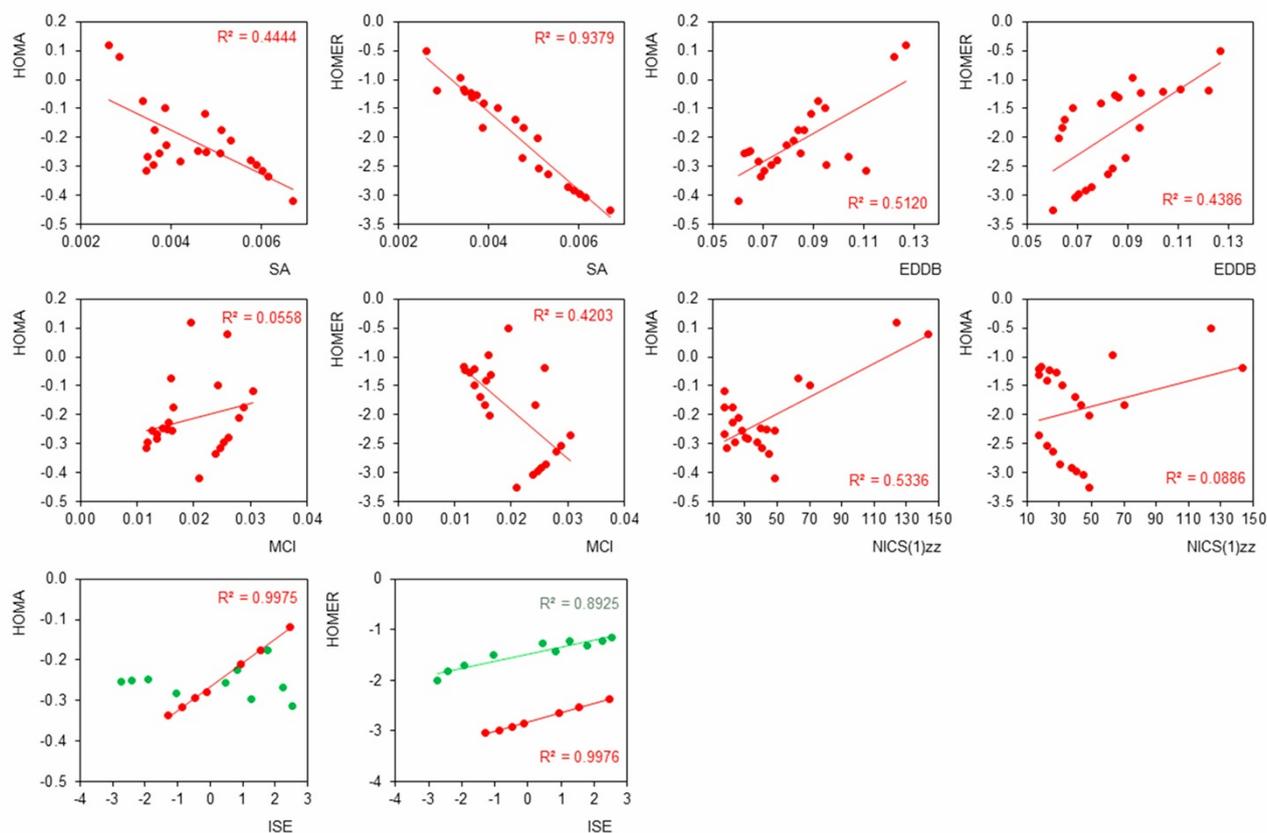

Figure S33. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI), NICS(1)$_{zz}$ and isomerization stabilization energy (ISE) calculated for five-membered rings of polycycles composed of benzene ring(s) and pentalene core in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. Pentalene is included in correlations, except for ISE when R^2 values decrease to 0.8762 and 0.8572 for HOMA and HOMER, respectively. For ISE, red color is used for correlations that involve the outer ring and green color for correlations that involve the inner ring (also see Figure S42).
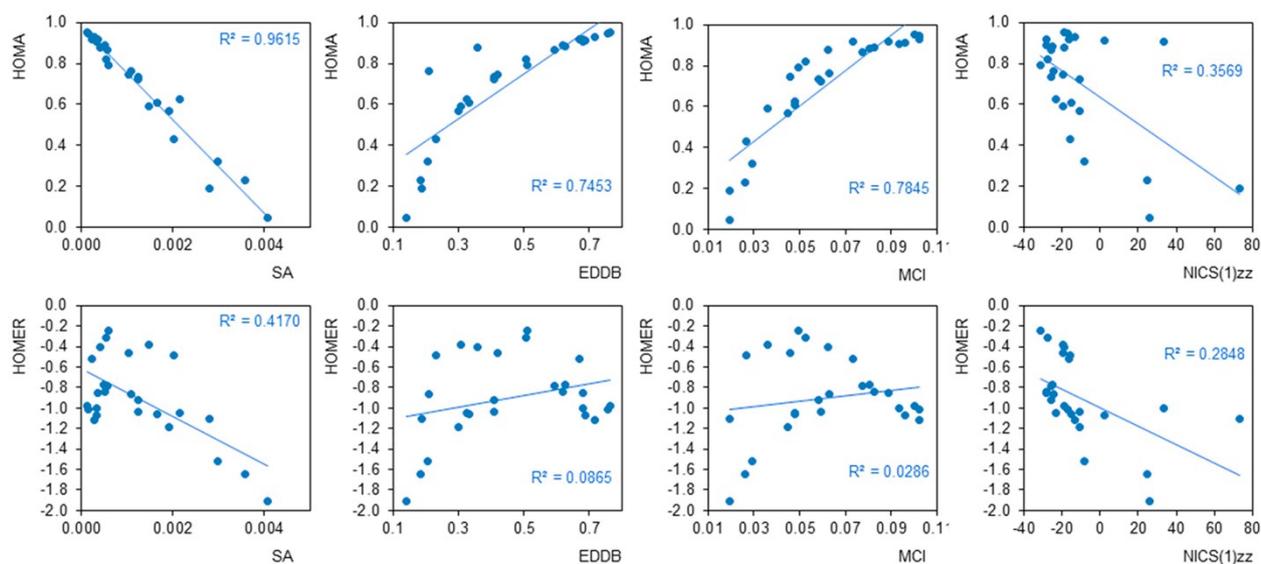
Figure S34. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and NICS(1)$_{zz}$ calculated for benzene subunits of polycycles composed of benzene ring(s) and pentalene core in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory.
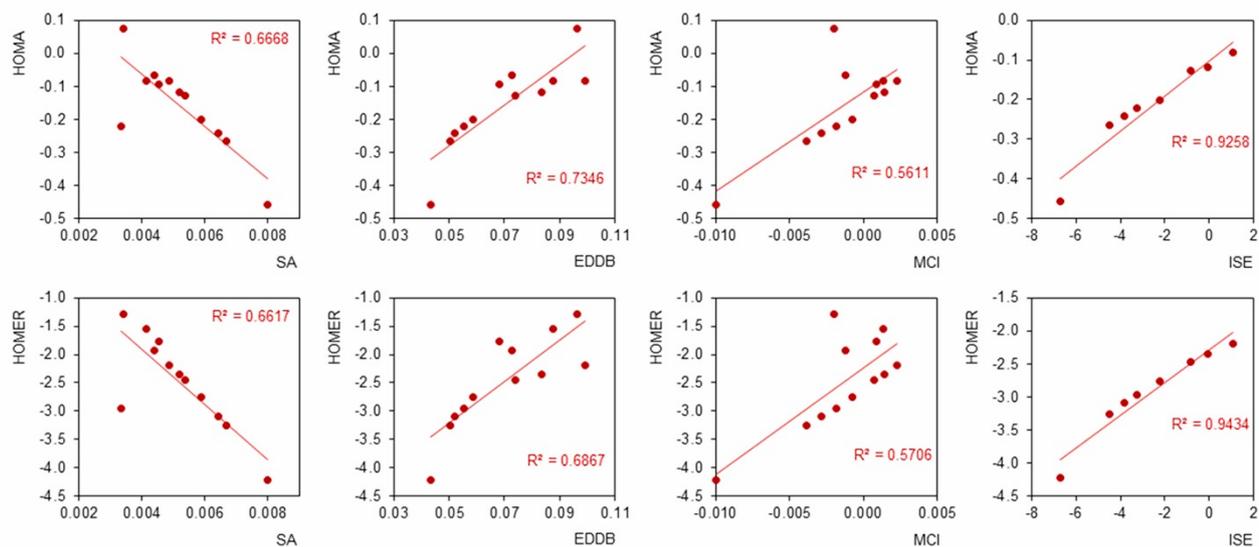
Figure S35. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB), multicenter index (MCI) and isomerization stabilization energy (ISE) calculated for perimeter of pentalene subunits of polycycles composed of benzene ring(s) and pentalene core in their S_0 state. Calculations were performed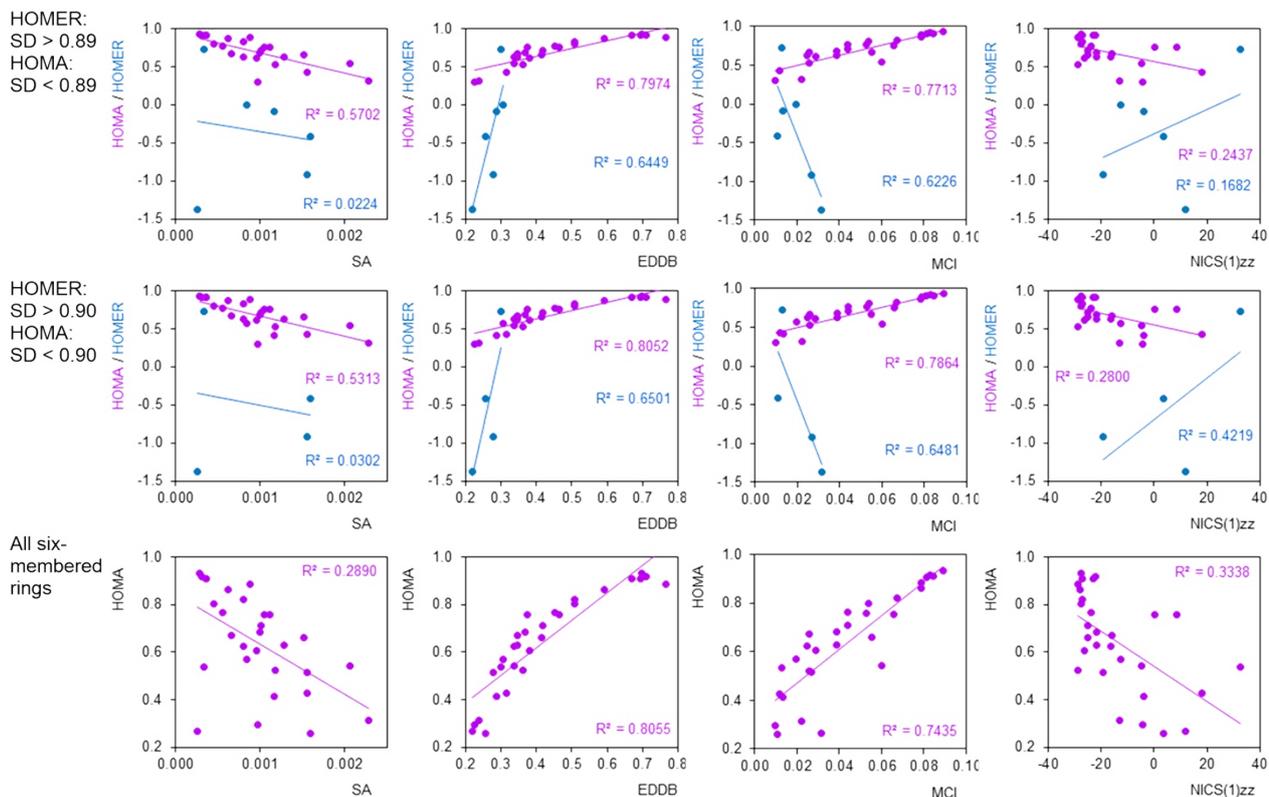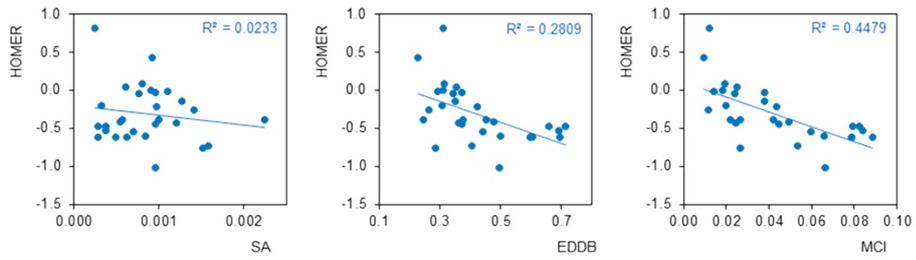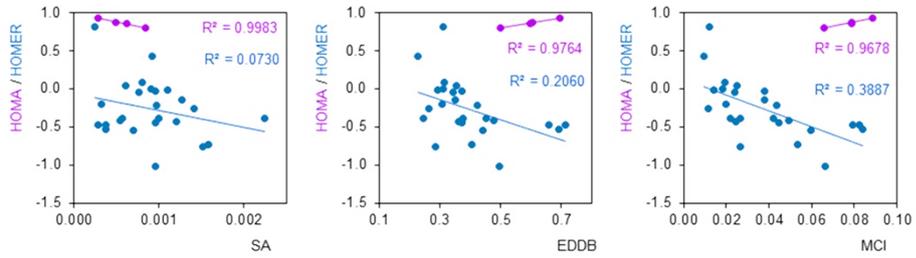 at the CAM-B3LYP/6-311+G(d,p) level of theory. Pentalene is included in correlations. The systems involved in correlations with ISE are shown in Figure S43.
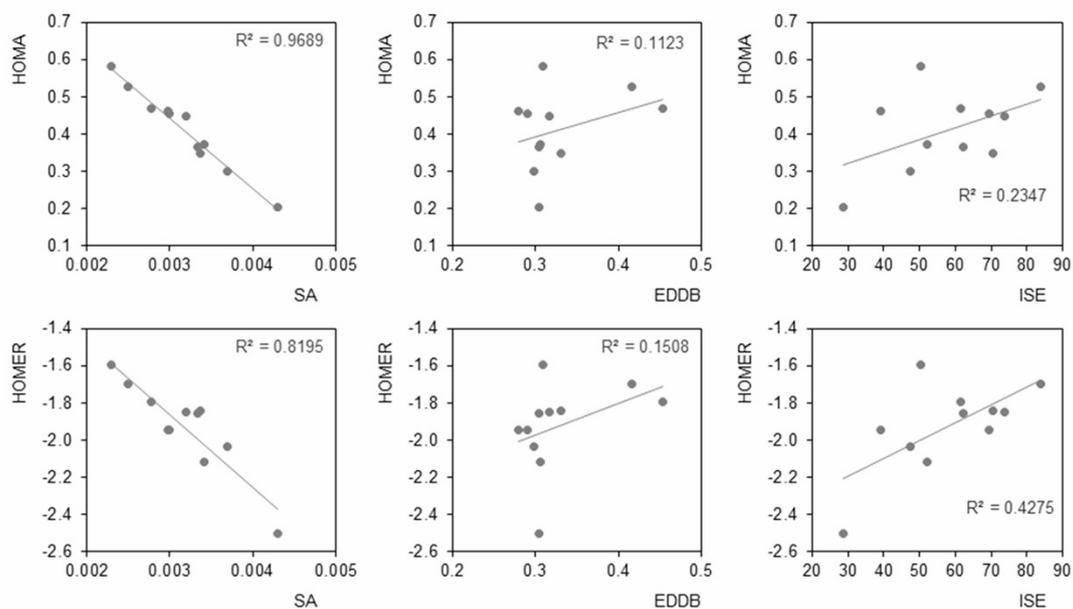
Figure S36. Correlations between HOMA/HOMER and Shannon aromaticity (SA), electron density of delocalized bonds per atom (EDDB) and isomerization stabilization energy (ISE) calculated for molecular perimeter of polycycles composed of benzene ring(s) and pentalene core in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. ISE schemes are shown in Figure S44.
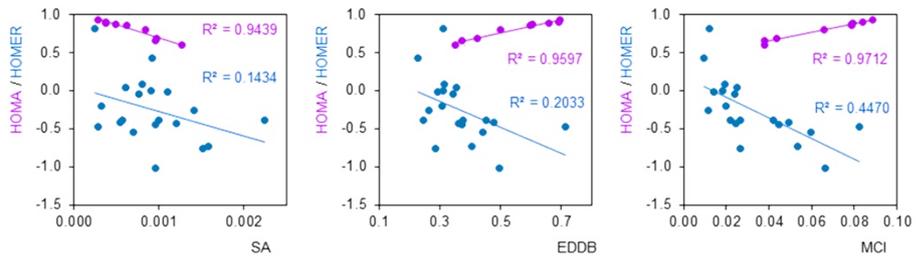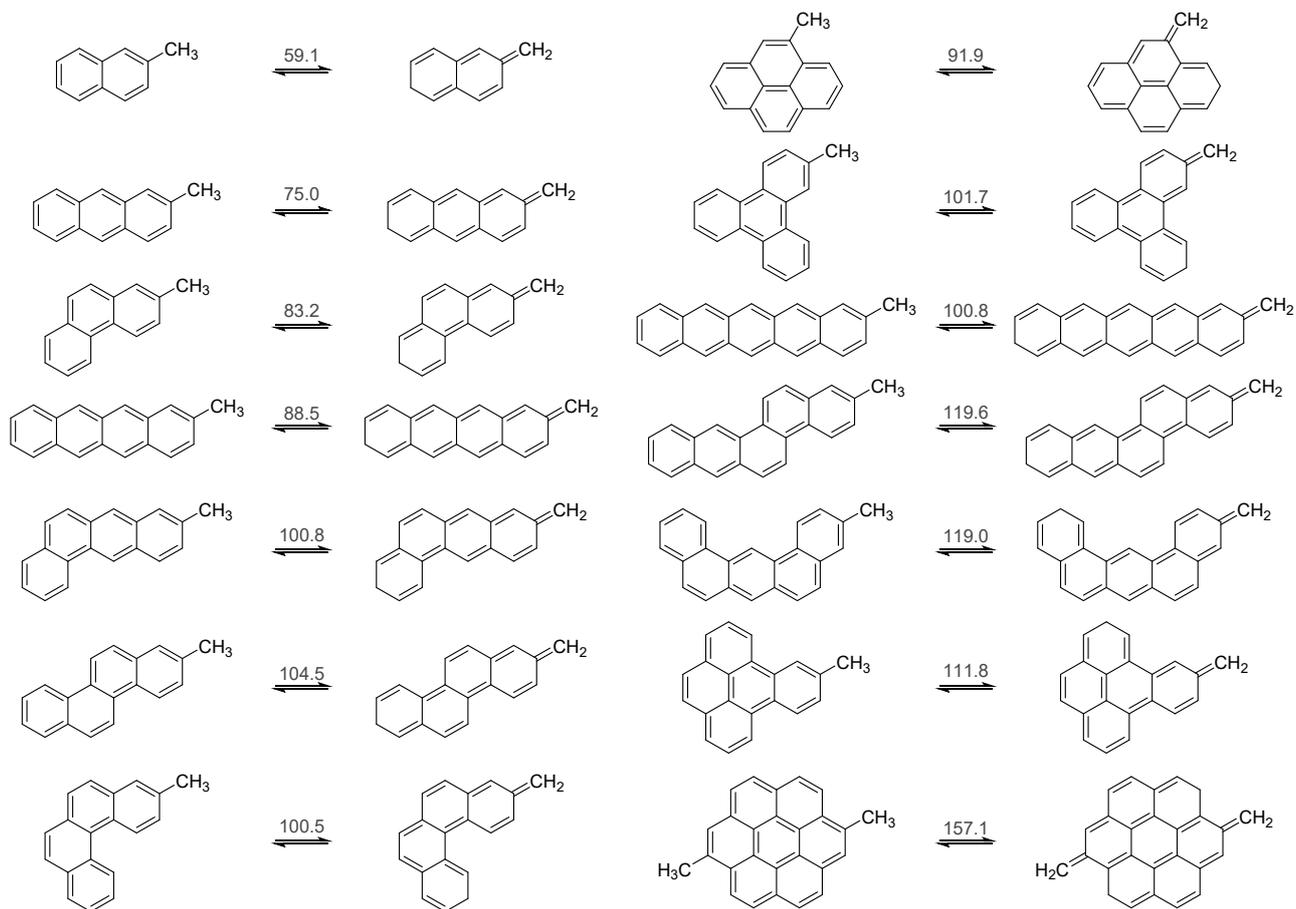
Figure S37. Calculated values of isomerization stabilization energies (kcal/mol) used to study the (anti)aromaticity of molecular perimeter of the given systems in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. Values include ZPE correction and correction for *syn/anti* mismatch.
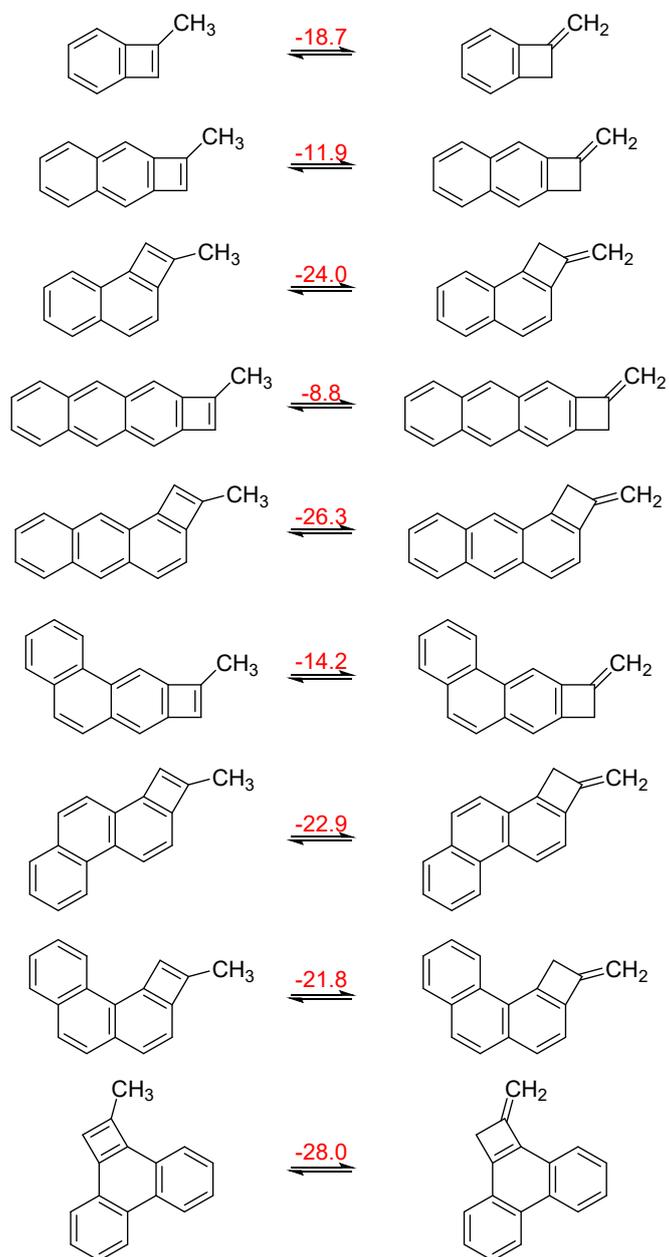
Figure S38. Calculated values of isomerization stabilization energies (kcal/mol) used to study the antiaromaticity of cyclobutadiene subunits of the given systems in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. Values include ZPE correction.
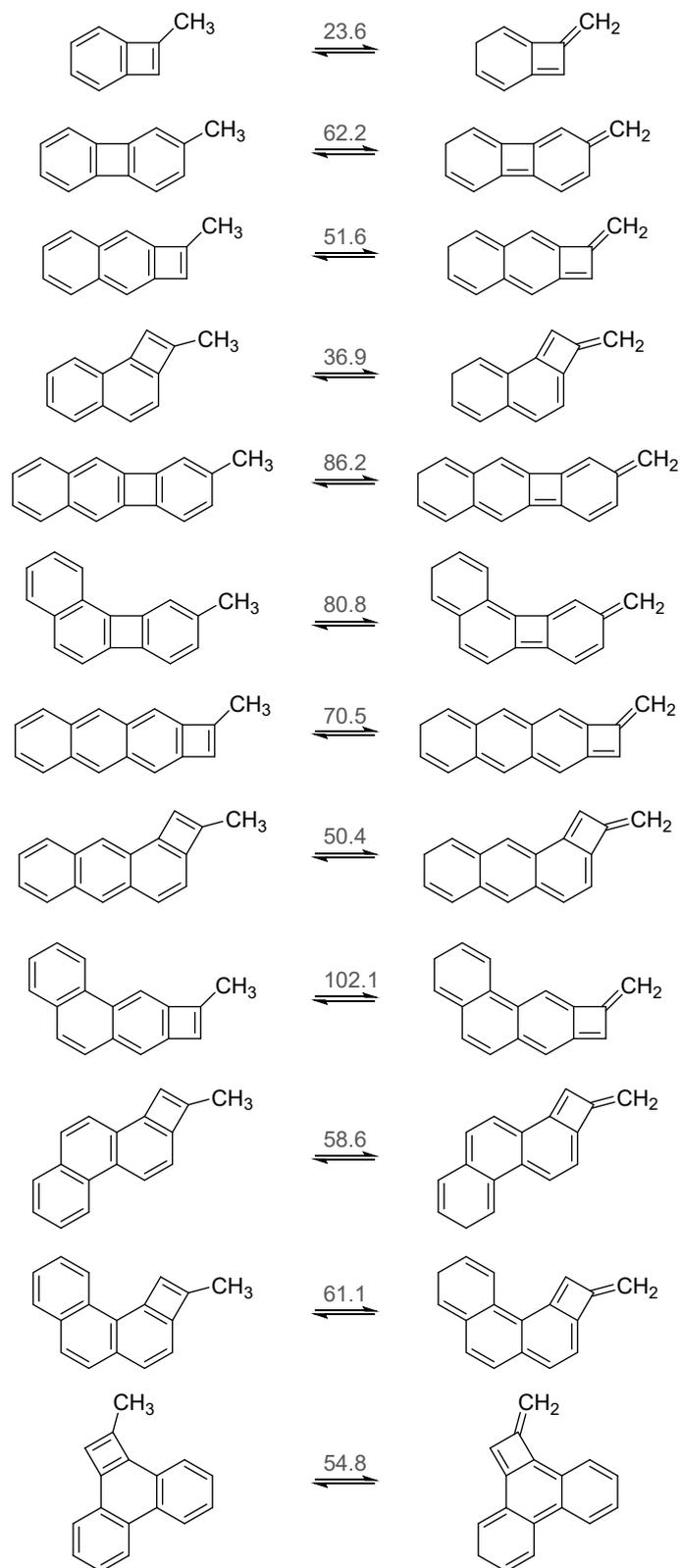
Figure S39. Calculated values of isomerization stabilization energies (kcal/mol) used to study the (anti)aromaticity of molecular perimeter of the given systems in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. Values include ZPE correction and correction for *syn/anti* mismatch.
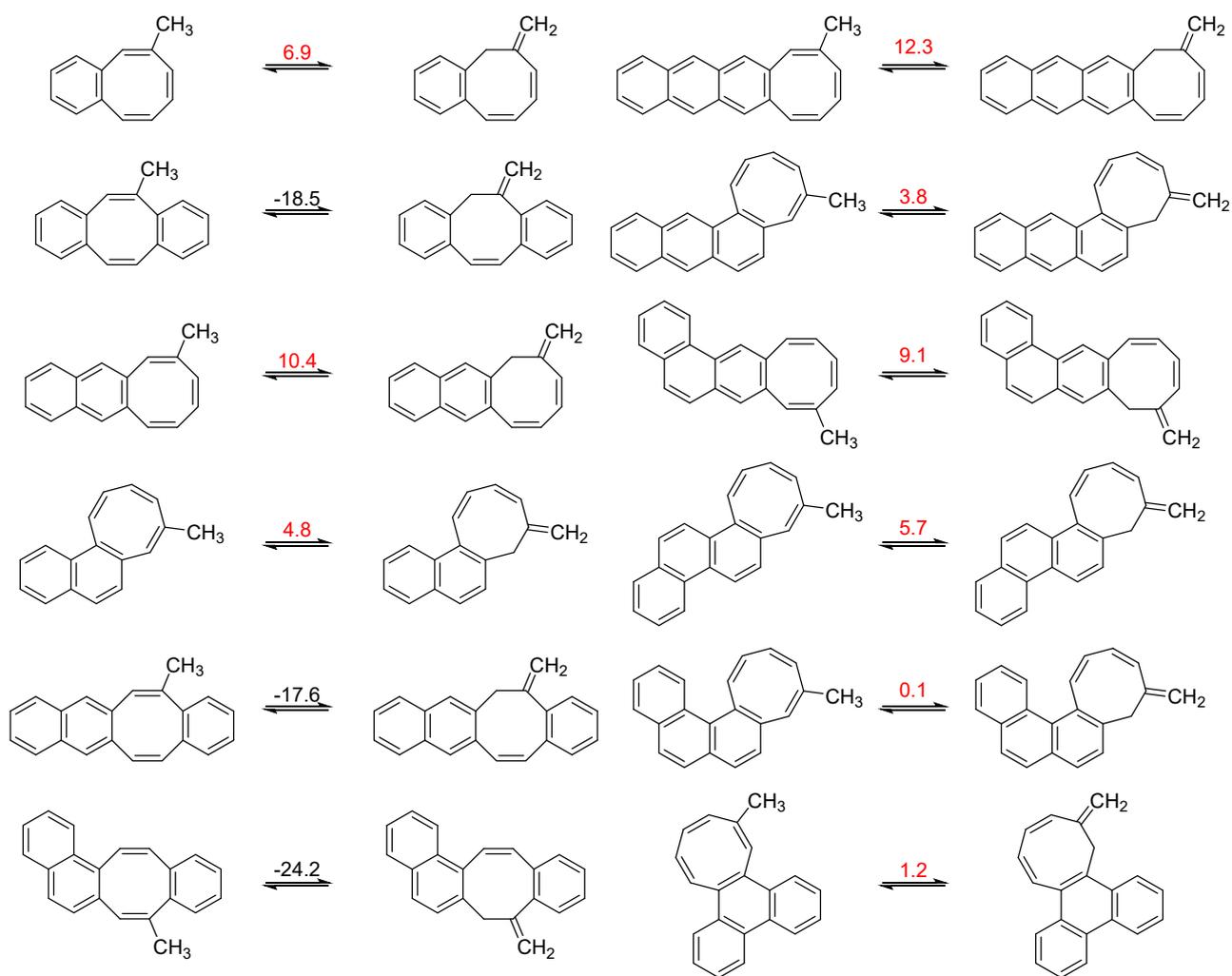
Figure S40. Calculated values of isomerization stabilization energies (kcal/mol) used to study the (anti)aromaticity of cyclooctatetraene subunits of the given systems in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. Values in black are for systems for which methylene isomers are nonplanar, but methyl isomers are planar. They are not included in correlations. Values include ZPE correction.
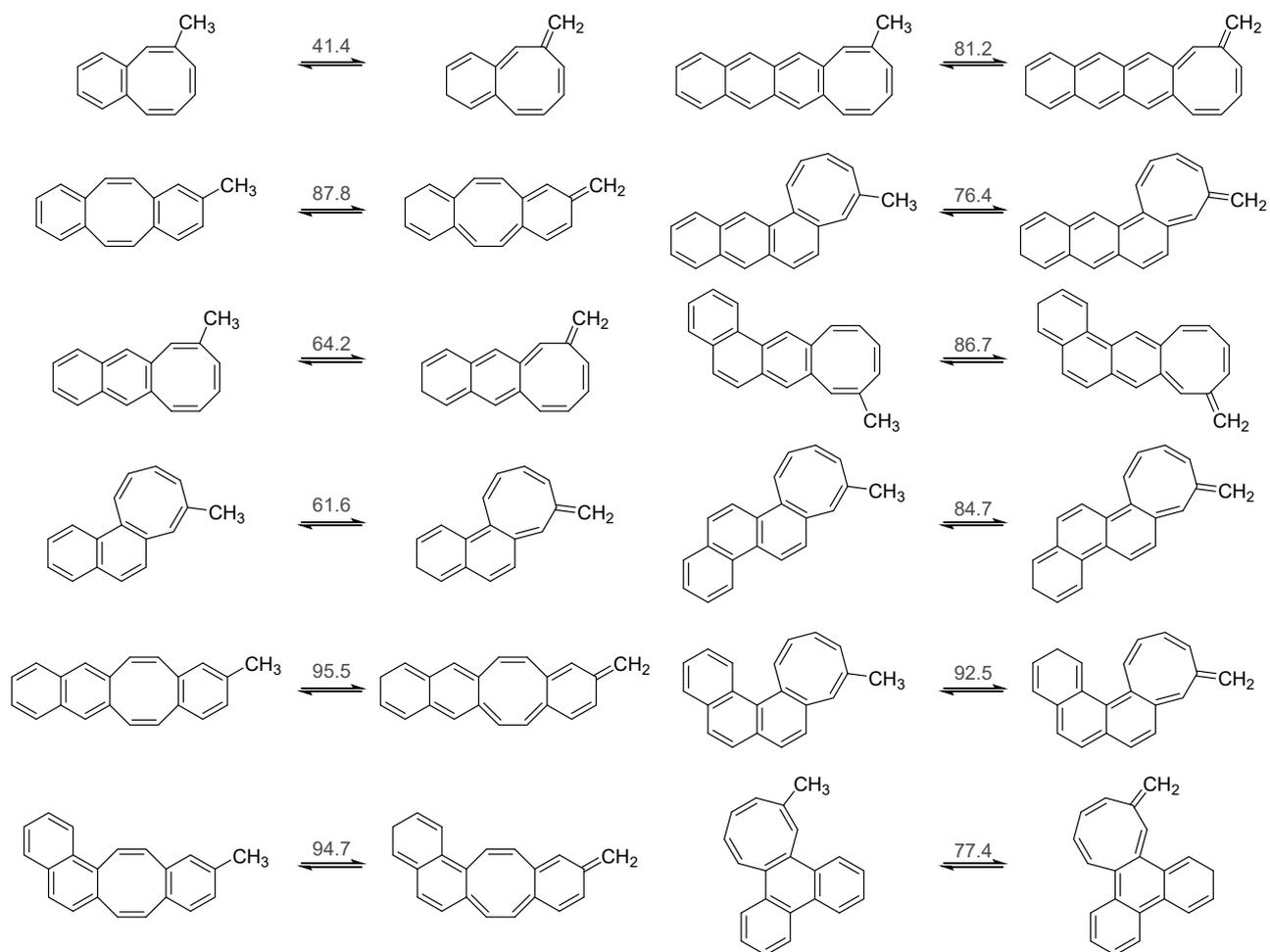
Figure S41. Calculated values of isomerization stabilization energies (kcal/mol) used to study the (anti)aromaticity of molecular perimeter of the given systems in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. Values include ZPE correction and correction for *syn/anti* mismatch.
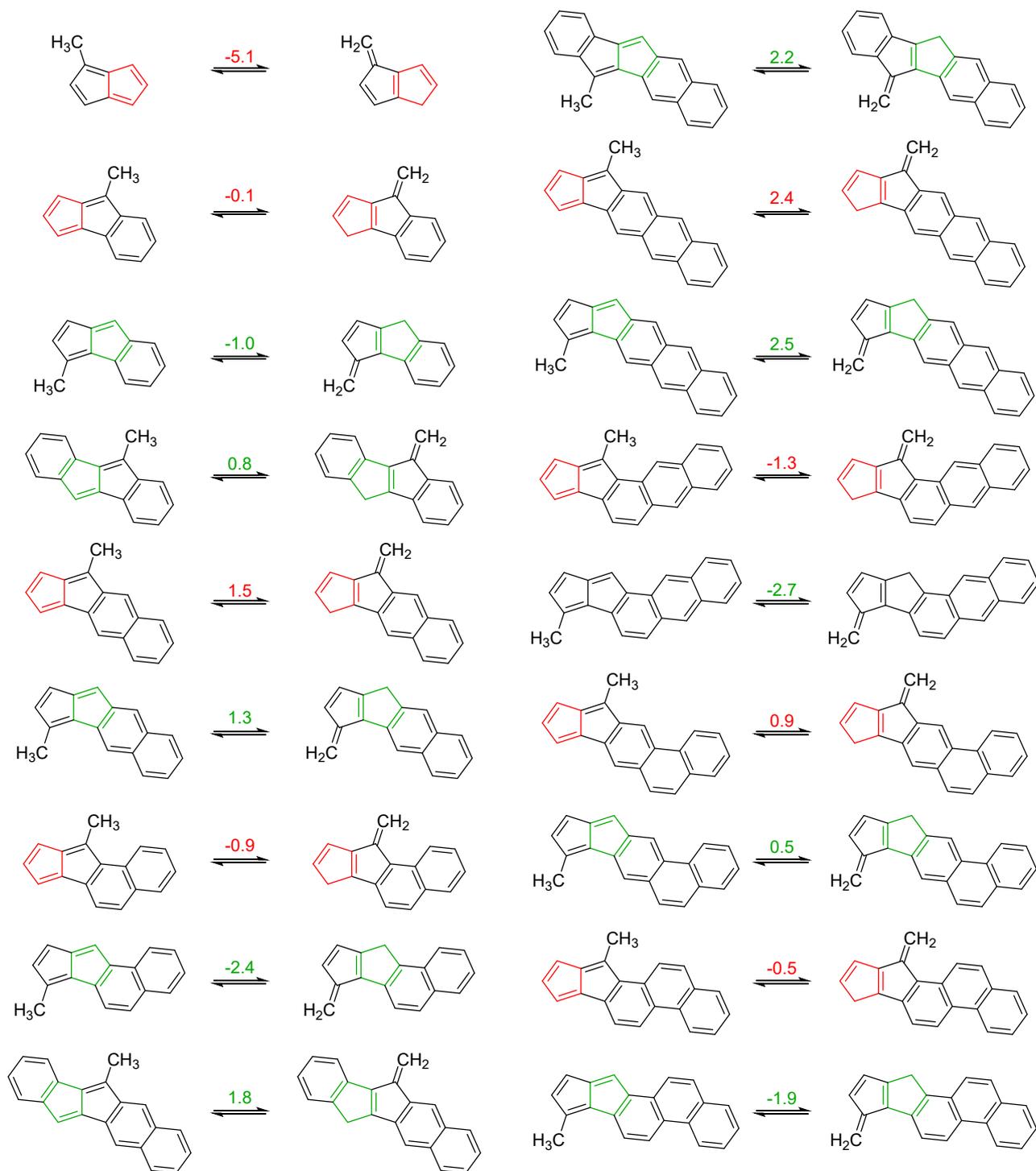
Figure S42. Calculated values of isomerization stabilization energies (kcal/mol) used to study delocalization in five-membered rings of the given systems in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. The color code corresponds to the graphs in Figure S33. Values include ZPE correction.
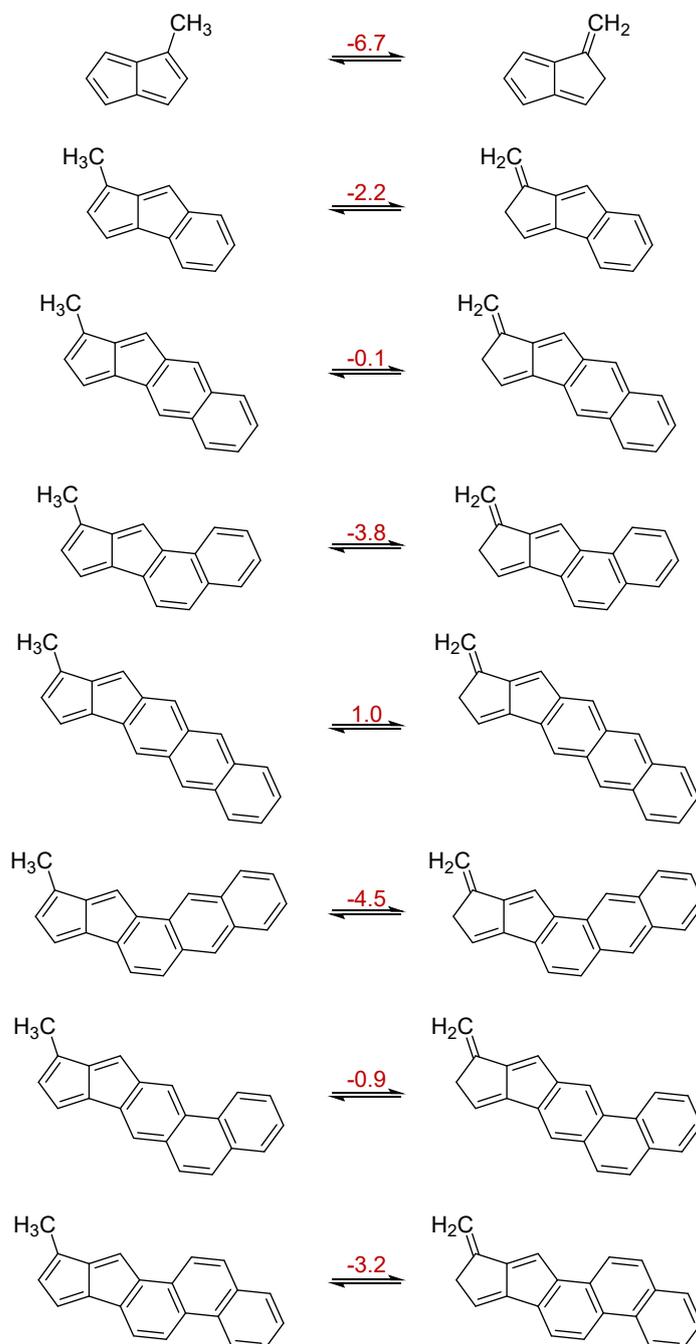
Figure S43. Calculated values of isomerization stabilization energies (kcal/mol) used to study the (anti)aromaticity of the perimeter of pentalene subunits of the given systems in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. Values include ZPE correction.
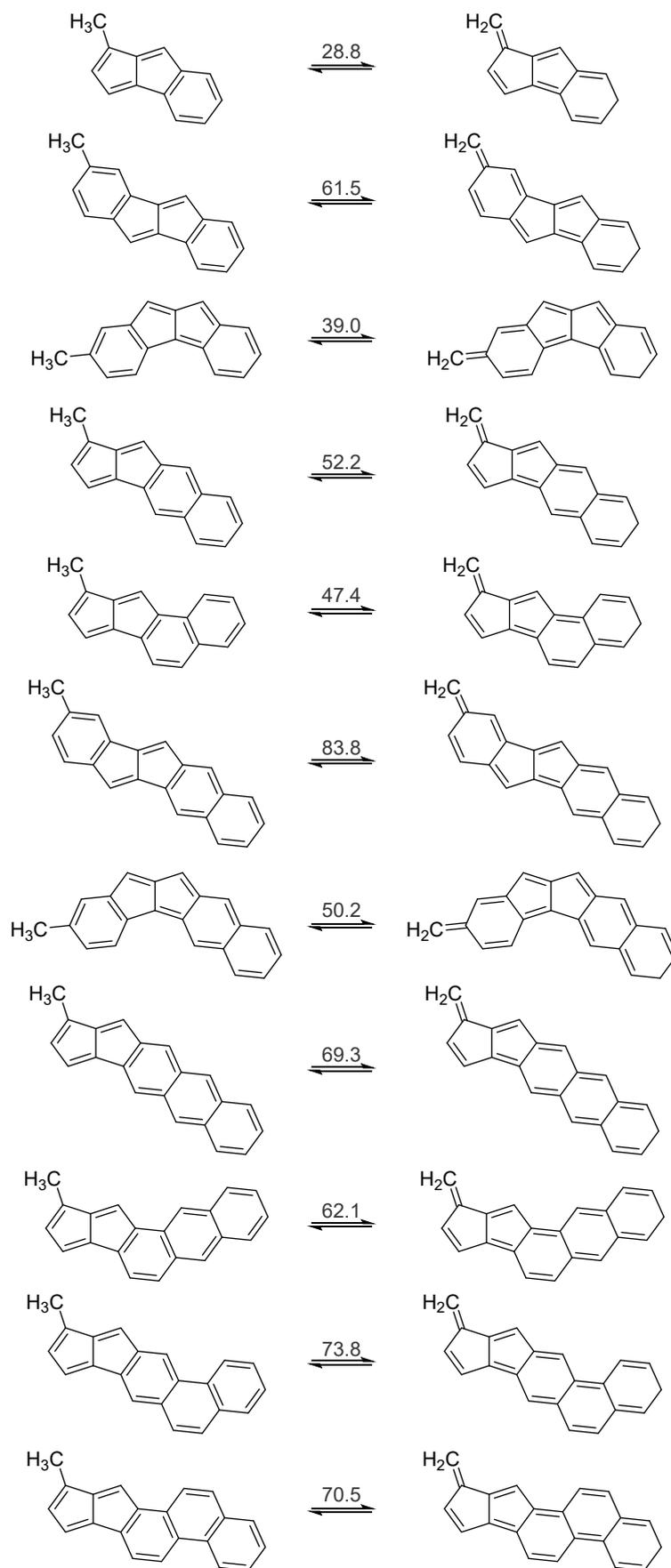
Figure S44. Calculated values of isomerization stabilization energies (kcal/mol) used to study the (anti)aromaticity of molecular perimeter of the given systems in their S_0 state. Calculations were performed at the CAM-B3LYP/6-311+G(d,p) level of theory. Values include ZPE correction and correction for *syn/anti* mismatch.

Absolute energies and x, y, z coordinates of optimized structures (CAM-B3LYP)

| | S₀ | | | | | T₁ | | | |

S_0

E = -385.7563652 a.u.

T_1

E = -385.6541843 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	-2.420483	-0.706171
2	6	0	0.000000	-1.240379	-1.394667
3	6	0	0.000000	0.000000	-0.709946
4	6	0	0.000000	0.000000	0.709946
5	6	0	0.000000	-1.240379	1.394667
6	6	0	0.000000	-2.420483	0.706171
7	1	0	0.000000	1.237653	-2.479206
8	1	0	0.000000	-3.362251	-1.242001
9	1	0	0.000000	-1.237653	-2.479206
10	6	0	0.000000	1.240379	-1.394667
11	6	0	0.000000	1.240379	1.394667
12	1	0	0.000000	-1.237653	2.479206
13	1	0	0.000000	-3.362251	1.242001
14	6	0	0.000000	2.420483	0.706171
15	6	0	0.000000	2.420483	-0.706171
16	1	0	0.000000	1.237653	2.479206
17	1	0	0.000000	3.362251	1.242001
18	1	0	0.000000	3.362251	-1.242001

T₁ (E = -385.6541843 a.u.)

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	-2.476080	0.675677
2	6	0	0.000000	-1.229032	1.395385
3	6	0	0.000000	0.000000	0.724424
4	6	0	0.000000	0.000000	-0.724424
5	6	0	0.000000	-1.229032	-1.395385
6	6	0	0.000000	-2.476080	-0.675677
7	1	0	0.000000	1.238282	2.478889
8	1	0	0.000000	-3.405841	1.230932
9	1	0	0.000000	-1.238282	2.478889
10	6	0	0.000000	1.229032	1.395385
11	6	0	0.000000	1.229032	-1.395385
12	1	0	0.000000	-1.238282	-2.478889
13	1	0	0.000000	-3.405841	-1.230932
14	6	0	0.000000	2.476080	-0.675677
15	6	0	0.000000	2.476080	0.675677
16	1	0	0.000000	1.238282	-2.478889
17	1	0	0.000000	3.405841	-1.230932
18	1	0	0.000000	3.405841	1.230932

S_0

E = -539.3383147 a.u.

T_1

E = -539.2696547 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	3.640846	-0.711893
2	6	0	0.000000	2.469850	-1.400059
3	6	0	0.000000	1.216004	-0.716057
4	6	0	0.000000	1.216004	0.716057
5	6	0	0.000000	2.469850	1.400059
6	6	0	0.000000	3.640846	0.711893
7	6	0	0.000000	0.000000	-1.394822
8	6	0	0.000000	0.000000	1.394822
9	6	0	0.000000	-1.216004	0.716057
10	6	0	0.000000	-1.216004	-0.716057
11	6	0	0.000000	-2.469850	-1.400059
12	1	0	0.000000	-2.467890	-2.484390
13	6	0	0.000000	-3.640846	-0.711893
14	6	0	0.000000	-3.640846	0.711893
15	6	0	0.000000	-2.469850	1.400059
16	1	0	0.000000	0.000000	-2.480048
17	1	0	0.000000	4.584788	-1.243722
18	1	0	0.000000	2.467890	-2.484390
19	1	0	0.000000	2.467890	2.484390
20	1	0	0.000000	4.584788	1.243722
21	1	0	0.000000	0.000000	2.480048
22	1	0	0.000000	-4.584788	-1.243722
23	1	0	0.000000	-4.584788	1.243722
24	1	0	0.000000	-2.467890	2.484390

T₁ (E = -539.2696547 a.u.)

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	3.687249	0.686783
2	6	0	0.000000	2.467294	1.387698
3	6	0	0.000000	1.253682	0.715950
4	6	0	0.000000	1.253682	-0.715950
5	6	0	0.000000	2.467294	-1.387698
6	6	0	0.000000	3.687249	-0.686783
7	6	0	0.000000	0.000000	1.404094
8	6	0	0.000000	0.000000	-1.404094
9	6	0	0.000000	-1.253682	-0.715950
10	6	0	0.000000	-1.253682	0.715950
11	6	0	0.000000	-2.467294	1.387698
12	1	0	0.000000	-2.470730	2.472014
13	6	0	0.000000	-3.687249	0.686783
14	6	0	0.000000	-3.687249	-0.686783
15	6	0	0.000000	-2.467294	-1.387698
16	1	0	0.000000	0.000000	2.488199
17	1	0	0.000000	4.620960	1.235679
18	1	0	0.000000	2.470730	2.472014
19	1	0	0.000000	2.470730	-2.472014
20	1	0	0.000000	4.620960	-1.235679
21	1	0	0.000000	0.000000	-2.488199
22	1	0	0.000000	-4.620960	1.235679
23	1	0	0.000000	-4.620960	-1.235679
24	1	0	0.000000	-2.470730	-2.472014

			S₀		

S₀
E = -539.3483794 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	-3.542189	-0.295723
2	6	0	0.000000	-2.823420	0.872430
3	6	0	0.000000	-1.415167	0.858773
4	6	0	0.000000	-0.727515	-0.375118
5	6	0	0.000000	-1.492005	-1.558350
6	6	0	0.000000	-2.865402	-1.522976
7	6	0	0.000000	-0.673941	2.086474
8	6	0	0.000000	0.727515	-0.375118
9	6	0	0.000000	1.415167	0.858773
10	6	0	0.000000	0.673941	2.086474
11	6	0	0.000000	2.823420	0.872430
12	1	0	0.000000	3.333000	1.829713
13	6	0	0.000000	3.542189	-0.295723
14	6	0	0.000000	2.865402	-1.522976
15	6	0	0.000000	1.492005	-1.558350
16	1	0	0.000000	-1.225983	3.019702
17	1	0	0.000000	-4.625215	-0.272620
18	1	0	0.000000	-3.333000	1.829713
19	1	0	0.000000	-0.998312	-2.520558
20	1	0	0.000000	-3.427329	-2.449304
21	1	0	0.000000	1.225983	3.019702
22	1	0	0.000000	4.625215	-0.272620
23	1	0	0.000000	3.427329	-2.449304
24	1	0	0.000000	0.998312	-2.520558

T₁
E = -539.2442546 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
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2	6	0	0.000000	-2.871144	0.870534
3	6	0	0.000000	-1.444439	0.882778
4	6	0	0.000000	-0.746797	-0.380796
5	6	0	0.000000	-1.489241	-1.536714
6	6	0	0.000000	-2.897030	-1.523425
7	6	0	0.000000	-0.739334	2.069287
8	6	0	0.000000	0.746797	-0.380796
9	6	0	0.000000	1.444439	0.882778
10	6	0	0.000000	0.739334	2.069287
11	6	0	0.000000	2.871144	0.870534
12	1	0	0.000000	3.391764	1.821273
13	6	0	0.000000	3.578614	-0.311782
14	6	0	0.000000	2.897030	-1.523425
15	6	0	0.000000	1.489241	-1.536714
16	1	0	0.000000	-1.267043	3.014421
17	1	0	0.000000	-4.661927	-0.295803
18	1	0	0.000000	-3.391764	1.821273
19	1	0	0.000000	-0.995232	-2.499424
20	1	0	0.000000	-3.440404	-2.459759
21	1	0	0.000000	1.267043	3.014421
22	1	0	0.000000	4.661927	-0.295803
23	1	0	0.000000	3.440404	-2.459759
24	1	0	0.000000	0.995232	-2.499424

S₀
E = -692.9173033 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	4.862380	0.715030
2	6	0	0.000000	3.695826	1.403111
3	6	0	0.000000	2.435183	0.720163
4	6	0	0.000000	2.435183	-0.720163
5	6	0	0.000000	3.695826	-1.403111
6	6	0	0.000000	4.862380	-0.715030
7	6	0	0.000000	1.230529	1.397979
8	6	0	0.000000	1.230529	-1.397979
9	6	0	0.000000	0.000000	-0.719095
10	6	0	0.000000	0.000000	0.719095
11	6	0	0.000000	-1.230529	1.397979
12	1	0	0.000000	-1.230450	2.483004
13	6	0	0.000000	-2.435183	0.720163
14	6	0	0.000000	-2.435183	-0.720163
15	6	0	0.000000	-1.230529	-1.397979
16	1	0	0.000000	1.230450	2.483004
17	1	0	0.000000	5.807693	1.244252
18	1	0	0.000000	3.693788	2.487375
19	1	0	0.000000	3.693788	-2.487375
20	1	0	0.000000	5.807693	-1.244252

T₁
E = -692.8716412 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
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2	6	0	0.000000	-3.698034	1.388711
3	6	0	0.000000	-2.478205	0.710589
4	6	0	0.000000	-2.478205	-0.710589
5	6	0	0.000000	-3.698034	-1.388711
6	6	0	0.000000	-4.900980	-0.694563
7	6	0	0.000000	-1.222255	1.400567
8	6	0	0.000000	-1.222255	-1.400567
9	6	0	0.000000	0.000000	-0.730768
10	6	0	0.000000	0.000000	0.730768
11	6	0	0.000000	1.222255	1.400567
12	1	0	0.000000	1.229117	2.485253
13	6	0	0.000000	2.478205	0.710589
14	6	0	0.000000	2.478205	-0.710589
15	6	0	0.000000	1.222255	-1.400567
16	1	0	0.000000	-1.229117	2.485253
17	1	0	0.000000	-5.837729	1.238410
18	1	0	0.000000	-3.698413	2.473081
19	1	0	0.000000	-3.698413	-2.473081
20	1	0	0.000000	-5.837729	-1.238410

21	1	0	0.000000	1.230450	-2.483004
22	1	0	0.000000	-1.230450	-2.483004
23	6	0	0.000000	-3.695826	-1.403111
24	1	0	0.000000	-3.693788	-2.487375
25	6	0	0.000000	-3.695826	1.403111
26	1	0	0.000000	-3.693788	2.487375
27	6	0	0.000000	-4.862380	-0.715030
28	1	0	0.000000	-5.807693	-1.244252
29	6	0	0.000000	-4.862380	0.715030
30	1	0	0.000000	-5.807693	1.244252

21	1	0	0.000000	-1.229117	-2.485253
22	1	0	0.000000	1.229117	-2.485253
23	6	0	0.000000	3.698034	-1.388711
24	1	0	0.000000	3.698413	-2.473081
25	6	0	0.000000	3.698034	1.388711
26	1	0	0.000000	3.698413	2.473081
27	6	0	0.000000	4.900980	-0.694563
28	1	0	0.000000	5.837729	-1.238410
29	6	0	0.000000	4.900980	0.694563
30	1	0	0.000000	5.837729	1.238410
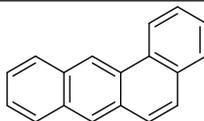
S_0						T_1					
E = -692.933219 a.u.						E = -692.852926 a.u.					
Center Number	Atomic Number	Atomic Type	X	Y	Z	Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-0.825731	-4.660796	0.000000	1	6	0	-0.491012	-4.751652	0.000000
2	6	0	0.306874	-3.905295	0.000000	2	6	0	0.611872	-3.869450	0.000000
3	6	0	0.233658	-2.483831	0.000000	3	6	0	0.429209	-2.491421	0.000000
4	6	0	-1.046114	-1.860137	0.000000	4	6	0	-0.906238	-1.967530	0.000000
5	6	0	-2.208019	-2.682648	0.000000	5	6	0	-1.971555	-2.849878	0.000000
6	6	0	-2.102293	-4.040126	0.000000	6	6	0	-1.764361	-4.251117	0.000000
7	6	0	1.372160	-1.670716	0.000000	7	6	0	1.508322	-1.573295	0.000000
8	6	0	-1.125976	-0.460588	0.000000	8	6	0	-1.091146	-0.548906	0.000000
9	6	0	0.000000	0.343773	0.000000	9	6	0	0.000000	0.377949	0.000000
10	6	0	1.283638	-0.289553	0.000000	10	6	0	1.308981	-0.139744	0.000000
11	6	0	2.473649	0.523000	0.000000	11	6	0	2.407489	0.727735	0.000000
12	1	0	3.434179	0.020301	0.000000	12	1	0	3.406600	0.306612	0.000000
13	6	0	2.402728	1.864574	0.000000	13	6	0	2.238704	2.094908	0.000000
14	6	0	1.133995	2.549110	0.000000	14	6	0	0.951177	2.654369	0.000000
15	6	0	-0.065401	1.806707	0.000000	15	6	0	-0.189952	1.792614	0.000000
16	1	0	2.352500	-2.135910	0.000000	16	1	0	2.524014	-1.951666	0.000000
17	1	0	-0.759344	-5.742145	0.000000	17	1	0	-0.320214	-5.821138	0.000000
18	1	0	1.283790	-4.375773	0.000000	18	1	0	1.619609	-4.269083	0.000000
19	1	0	-3.182305	-2.206613	0.000000	19	1	0	-2.983251	-2.459871	0.000000
20	1	0	-2.993741	-4.655775	0.000000	20	1	0	-2.618206	-4.917259	0.000000
21	1	0	-2.114035	-0.018686	0.000000	21	1	0	-2.109114	-0.186016	0.000000
22	1	0	3.305813	2.464533	0.000000	22	1	0	3.099992	2.752773	0.000000
23	6	0	1.084803	3.952537	0.000000	23	6	0	0.762438	4.062189	0.000000
24	1	0	2.017226	4.506130	0.000000	24	1	0	1.640038	4.699041	0.000000
25	6	0	-1.279181	2.513057	0.000000	25	6	0	-1.475155	2.401376	0.000000
26	1	0	-2.218109	1.976318	0.000000	26	1	0	-2.362767	1.784323	0.000000
27	6	0	-1.308797	3.890094	0.000000	27	6	0	-1.620103	3.758043	0.000000
28	1	0	-2.260946	4.406910	0.000000	28	1	0	-2.612529	4.192633	0.000000
29	6	0	-0.117236	4.620398	0.000000	29	6	0	-0.486509	4.605319	0.000000
30	1	0	-0.141571	5.703352	0.000000	30	1	0	-0.617135	5.680593	0.000000
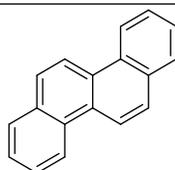
S_0						T_1					
E = -692.9374731 a.u.						E = -692.8399155 a.u.					
Center Number	Atomic Number	Atomic Type	X	Y	Z	Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-0.626039	2.490085	0.000000	1	6	0	-0.643785	2.519514	0.000000

2	6	0	0.607198	1.799107	0.000000
3	6	0	0.607198	0.350190	0.000000
4	6	0	-0.607198	-0.350190	0.000000
5	6	0	-1.828883	0.390332	0.000000
6	6	0	-1.838950	1.743132	0.000000
7	1	0	2.773093	0.134888	0.000000
8	6	0	1.828883	-0.390332	0.000000
9	6	0	-0.607198	-1.799107	0.000000
10	1	0	-2.773093	-0.134888	0.000000
11	1	0	-2.779664	2.282170	0.000000
12	6	0	0.626039	-2.490085	0.000000
13	6	0	1.838950	-1.743132	0.000000
14	1	0	2.779664	-2.282170	0.000000
15	6	0	-1.791711	-2.570026	0.000000
16	1	0	-2.757052	-2.083966	0.000000
17	6	0	0.642756	-3.900716	0.000000
18	1	0	1.601099	-4.408033	0.000000
19	6	0	-1.752300	-3.941208	0.000000
20	1	0	-2.677676	-4.504612	0.000000
21	6	0	-0.522948	-4.618953	0.000000
22	1	0	-0.500479	-5.701909	0.000000
23	6	0	-0.642756	3.900716	0.000000
24	1	0	-1.601099	4.408033	0.000000
25	6	0	1.791711	2.570026	0.000000
26	1	0	2.757052	2.083966	0.000000
27	6	0	1.752300	3.941208	0.000000
28	1	0	2.677676	4.504612	0.000000
29	6	0	0.522948	4.618953	0.000000
30	1	0	0.500479	5.701909	0.000000

2	6	0	0.611130	1.855545	0.000000
3	6	0	0.643785	0.369836	0.000000
4	6	0	-0.643785	-0.369836	0.000000
5	6	0	-1.806374	0.333896	0.000000
6	6	0	-1.841387	1.751365	0.000000
7	1	0	2.756130	0.183883	0.000000
8	6	0	1.806374	-0.333896	0.000000
9	6	0	-0.611130	-1.855545	0.000000
10	1	0	-2.756130	-0.183883	0.000000
11	1	0	-2.795153	2.263806	0.000000
12	6	0	0.643785	-2.519514	0.000000
13	6	0	1.841387	-1.751365	0.000000
14	1	0	2.795153	-2.263806	0.000000
15	6	0	-1.759893	-2.629904	0.000000
16	1	0	-2.734181	-2.159893	0.000000
17	6	0	0.683521	-3.920614	0.000000
18	1	0	1.648807	-4.414341	0.000000
19	6	0	-1.705788	-4.026028	0.000000
20	1	0	-2.626674	-4.596064	0.000000
21	6	0	-0.481898	-4.671837	0.000000
22	1	0	-0.431598	-5.753888	0.000000
23	6	0	-0.683521	3.920614	0.000000
24	1	0	-1.648807	4.414341	0.000000
25	6	0	1.759893	2.629904	0.000000
26	1	0	2.734181	2.159893	0.000000
27	6	0	1.705788	4.026028	0.000000
28	1	0	2.626674	4.596064	0.000000
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30	1	0	0.431598	5.753888	0.000000
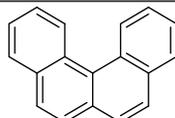
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2	6	0	0.000000	3.782990	-0.083933		2	6	0	0.000000	-3.762483	-0.079207
3	6	0	0.000000	2.495256	0.493197		3	6	0	0.000000	-2.501515	0.483555
4	6	0	0.000000	1.318628	-0.314303		4	6	0	0.000000	-1.316341	-0.334691
5	6	0	0.000000	1.566361	-1.711268		5	6	0	0.000000	-1.565569	-1.716464
6	6	0	0.000000	2.827974	-2.253440		6	6	0	0.000000	-2.852125	-2.272790
7	6	0	0.000000	2.408959	1.911966		7	6	0	0.000000	-2.408158	1.927534
8	6	0	0.000000	0.000000	0.339080		8	6	0	0.000000	0.000000	0.307074
9	6	0	0.000000	0.000000	1.749543		9	6	0	0.000000	0.000000	1.830567
10	6	0	0.000000	1.205550	2.510790		10	6	0	0.000000	-1.198448	2.548518
11	6	0	0.000000	-1.205550	2.510790		11	6	0	0.000000	1.198448	2.548518
12	1	0	0.000000	-1.123834	3.591185		12	1	0	0.000000	1.141165	3.631222
13	6	0	0.000000	-2.408959	1.911966		13	6	0	0.000000	2.408158	1.927534
14	6	0	0.000000	-2.495256	0.493197		14	6	0	0.000000	2.501515	0.483555
15	6	0	0.000000	-1.318628	-0.314303		15	6	0	0.000000	1.316341	-0.334691
16	1	0	0.000000	3.325053	2.490913		16	1	0	0.000000	-3.328319	2.498595
17	1	0	0.000000	4.956910	-1.869191		17	1	0	0.000000	-4.959220	-1.881720
18	1	0	0.000000	4.636904	0.584131		18	1	0	0.000000	-4.620555	0.583346
19	1	0	0.000000	0.767605	-2.420900		19	1	0	0.000000	-0.769408	-2.429176
20	1	0	0.000000	2.934427	-3.331759		20	1	0	0.000000	-2.952015	-3.351432
21	1	0	0.000000	1.123834	3.591185		21	1	0	0.000000	-1.141165	3.631222
22	1	0	0.000000	-3.325053	2.490913		22	1	0	0.000000	3.328319	2.498595
23	6	0	0.000000	-1.566361	-1.711268		23	6	0	0.000000	1.565569	-1.716464
24	1	0	0.000000	-0.767605	-2.420900		24	1	0	0.000000	0.769408	-2.429176
25	6	0	0.000000	-2.827974	-2.253440		25	6	0	0.000000	2.852125	-2.272790
26	1	0	0.000000	-2.934427	-3.331759		26	1	0	0.000000	2.952015	-3.351432
27	6	0	0.000000	-3.782990	-0.083933		27	6	0	0.000000	3.762483	-0.079207
28	1	0	0.000000	-4.636904	0.584131		28	1	0	0.000000	4.620555	0.583346

29	6	0	0.000000	-3.963457	-1.438050
30	1	0	0.000000	-4.956910	-1.869191

29	6	0	0.000000	3.958964	-1.467081
30	1	0	0.000000	4.959220	-1.881720
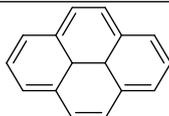
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1	6	0	0.000000	0.000000	-3.505433	1	6	0	0.000000	0.000000	3.542973
2	6	0	0.000000	1.203747	-2.817608	2	6	0	0.000000	1.204123	2.862309
3	6	0	0.000000	1.226887	-1.422460	3	6	0	0.000000	1.235967	1.416880
4	6	0	0.000000	0.000000	-0.712648	4	6	0	0.000000	0.000000	0.705215
5	6	0	0.000000	-1.226887	-1.422460	5	6	0	0.000000	-1.235967	1.416880
6	6	0	0.000000	-1.203747	-2.817608	6	6	0	0.000000	-1.204123	2.862309
7	6	0	0.000000	2.454353	-0.674611	7	6	0	0.000000	2.420300	0.703199
8	6	0	0.000000	0.000000	0.712648	8	6	0	0.000000	0.000000	-0.705215
9	6	0	0.000000	1.226887	1.422460	9	6	0	0.000000	1.235967	-1.416880
10	6	0	0.000000	2.454353	0.674611	10	6	0	0.000000	2.420300	-0.703199
11	6	0	0.000000	1.203747	2.817608	11	6	0	0.000000	1.204123	-2.862309
12	1	0	0.000000	2.141396	3.362137	12	1	0	0.000000	2.143502	-3.401608
13	6	0	0.000000	0.000000	3.505433	13	6	0	0.000000	0.000000	-3.542973
14	6	0	0.000000	-1.203747	2.817608	14	6	0	0.000000	-1.204123	-2.862309
15	6	0	0.000000	-1.226887	1.422460	15	6	0	0.000000	-1.235967	-1.416880
16	6	0	0.000000	-2.454353	0.674611	16	6	0	0.000000	-2.420300	-0.703199
17	6	0	0.000000	-2.454353	-0.674611	17	6	0	0.000000	-2.420300	0.703199
18	1	0	0.000000	-3.389849	-1.222960	18	1	0	0.000000	-3.363516	1.237467
19	1	0	0.000000	-3.389849	1.222960	19	1	0	0.000000	-3.363516	-1.237467
20	1	0	0.000000	3.389849	-1.222960	20	1	0	0.000000	3.363516	1.237467
21	1	0	0.000000	0.000000	-4.588982	21	1	0	0.000000	0.000000	4.626770
22	1	0	0.000000	2.141396	-3.362137	22	1	0	0.000000	2.143502	3.401608
23	1	0	0.000000	-2.141396	-3.362137	23	1	0	0.000000	-2.143502	3.401608
24	1	0	0.000000	3.389849	1.222960	24	1	0	0.000000	3.363516	-1.237467
25	1	0	0.000000	0.000000	4.588982	25	1	0	0.000000	0.000000	-4.626770
26	1	0	0.000000	-2.141396	3.362137	26	1	0	0.000000	-2.143502	-3.401608
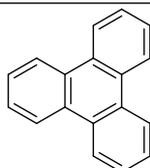
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Center Number	Atomic Number	Atomic Type	X	Y	Z	Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	1.376049	2.487542	0.000000	1	6	0	0.000000	1.390344	2.482491
2	6	0	0.703833	1.252867	0.000000	2	6	0	0.000000	0.701552	1.253129
3	6	0	1.436931	-0.016896	0.000000	3	6	0	0.000000	1.432248	0.003910
4	6	0	2.842299	-0.052078	0.000000	4	6	0	0.000000	2.833379	-0.034198
5	6	0	-0.703833	1.252867	0.000000	5	6	0	0.000000	-0.701552	1.253129
6	6	0	0.733098	-1.235971	0.000000	6	6	0	0.000000	0.709057	-1.235126
7	6	0	-0.733098	-1.235971	0.000000	7	6	0	0.000000	-0.709057	-1.235126
8	6	0	-1.436931	-0.016896	0.000000	8	6	0	0.000000	-1.432248	0.003910
9	6	0	-1.466250	-2.435464	0.000000	9	6	0	0.000000	-1.444726	-2.463315
10	6	0	1.466250	-2.435464	0.000000	10	6	0	0.000000	1.444726	-2.463315
11	6	0	2.841320	-2.445351	0.000000	11	6	0	0.000000	2.821089	-2.460448
12	6	0	3.538396	-1.237980	0.000000	12	6	0	0.000000	3.514004	-1.250006
13	1	0	4.621578	-1.229836	0.000000	13	1	0	0.000000	4.597621	-1.251980
14	1	0	3.375858	-3.387486	0.000000	14	1	0	0.000000	3.365212	-3.396635

15	6	0	0.697076	3.683331	0.000000		15	6	0	0.000000	0.682466	3.707773
16	6	0	-0.697076	3.683331	0.000000		16	6	0	0.000000	-0.682466	3.707773
17	6	0	-1.376049	2.487542	0.000000		17	6	0	0.000000	-1.390344	2.482491
18	1	0	1.245720	4.617322	0.000000		18	1	0	0.000000	1.233538	4.640248
19	1	0	-1.245720	4.617322	0.000000		19	1	0	0.000000	-1.233538	4.640248
20	6	0	-2.842299	-0.052078	0.000000		20	6	0	0.000000	-2.833379	-0.034198
21	6	0	-2.841320	-2.445351	0.000000		21	6	0	0.000000	-2.821089	-2.460448
22	1	0	-3.375858	-3.387486	0.000000		22	1	0	0.000000	-3.365212	-3.396635
23	6	0	-3.538396	-1.237980	0.000000		23	6	0	0.000000	-3.514004	-1.250006
24	1	0	-4.621578	-1.229836	0.000000		24	1	0	0.000000	-4.597621	-1.251980
25	1	0	-0.950150	-3.384392	0.000000		25	1	0	0.000000	-0.924705	-3.406464
26	1	0	-3.406044	0.869342	0.000000		26	1	0	0.000000	-3.406793	0.878237
27	1	0	-2.455894	2.515050	0.000000		27	1	0	0.000000	-2.467880	2.511332
28	1	0	2.455894	2.515050	0.000000		28	1	0	0.000000	2.467880	2.511332
29	1	0	0.950150	-3.384392	0.000000		29	1	0	0.000000	0.924705	-3.406464
30	1	0	3.406044	0.869342	0.000000		30	1	0	0.000000	3.406793	0.878237

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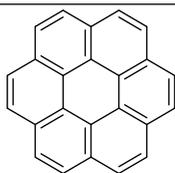
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1	6	0	-1.244095	-3.516569	0.000000		1	6	0	0.000000	3.510355	1.236157
2	6	0	0.000000	-2.831001	0.000000		2	6	0	0.000000	2.833808	0.000000
3	6	0	0.000000	-1.423340	0.000000		3	6	0	0.000000	1.408015	0.000000
4	6	0	-1.232606	-0.711664	0.000000		4	6	0	0.000000	0.700390	1.225819
5	6	0	-2.451643	-1.415521	0.000000		5	6	0	0.000000	1.429857	2.473541
6	6	0	-2.423293	-2.835727	0.000000		6	6	0	0.000000	2.805966	2.446480
7	6	0	1.232606	-0.711664	0.000000		7	6	0	0.000000	0.700390	-1.225819
8	6	0	-1.232606	0.711664	0.000000		8	6	0	0.000000	-0.700390	1.225819
9	6	0	0.000000	1.423340	0.000000		9	6	0	0.000000	-1.408015	0.000000
10	6	0	1.232606	0.711664	0.000000		10	6	0	0.000000	-0.700390	-1.225819
11	6	0	0.000000	2.831001	0.000000		11	6	0	0.000000	-2.833808	0.000000
12	6	0	-1.244095	3.516569	0.000000		12	6	0	0.000000	-3.510355	1.236157
13	6	0	-2.423293	2.835727	0.000000		13	6	0	0.000000	-2.805966	2.446480
14	6	0	-2.451643	1.415521	0.000000		14	6	0	0.000000	-1.429857	2.473541
15	6	0	-3.667386	0.680816	0.000000		15	6	0	0.000000	-0.670531	3.711584
16	6	0	-3.667386	-0.680816	0.000000		16	6	0	0.000000	0.670531	3.711584
17	1	0	-4.604421	-1.226371	0.000000		17	1	0	0.000000	1.222107	4.645022
18	1	0	-4.604421	1.226371	0.000000		18	1	0	0.000000	-1.222107	4.645022
19	1	0	-1.240058	-4.600833	0.000000		19	1	0	0.000000	4.593845	1.242048
20	1	0	-3.364265	-3.374464	0.000000		20	1	0	0.000000	3.354642	3.381821
21	1	0	-1.240058	4.600833	0.000000		21	1	0	0.000000	-4.593845	1.242048
22	1	0	-3.364265	3.374464	0.000000		22	1	0	0.000000	-3.354642	3.381821
23	6	0	1.244095	-3.516569	0.000000		23	6	0	0.000000	3.510355	-1.236157
24	6	0	2.423293	-2.835727	0.000000		24	6	0	0.000000	2.805966	-2.446480
25	6	0	2.451643	-1.415521	0.000000		25	6	0	0.000000	1.429857	-2.473541
26	1	0	1.240058	-4.600833	0.000000		26	1	0	0.000000	4.593845	-1.242048
27	1	0	3.364265	-3.374464	0.000000		27	1	0	0.000000	3.354642	-3.381821
28	6	0	3.667386	-0.680816	0.000000		28	6	0	0.000000	0.670531	-3.711584
29	6	0	3.667386	0.680816	0.000000		29	6	0	0.000000	-0.670531	-3.711584
30	6	0	2.451643	1.415521	0.000000		30	6	0	0.000000	-1.429857	-2.473541
31	1	0	4.604421	-1.226371	0.000000		31	1	0	0.000000	1.222107	-4.645022
32	1	0	4.604421	1.226371	0.000000		32	1	0	0.000000	-1.222107	-4.645022
33	6	0	1.244095	3.516569	0.000000		33	6	0	0.000000	-3.510355	-1.236157
34	1	0	1.240058	4.600833	0.000000		34	1	0	0.000000	-4.593845	-1.242048
35	6	0	2.423293	2.835727	0.000000		35	6	0	0.000000	-2.805966	-2.446480
36	1	0	3.364265	3.374464	0.000000		36	1	0	0.000000	-3.354642	-3.381821

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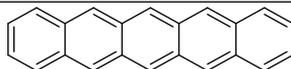
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3	6	0	0.000000	1.218634	0.721788
4	6	0	0.000000	1.218634	-0.721788
5	6	0	0.000000	2.457570	-1.400029
6	6	0	0.000000	3.656098	-0.722793
7	6	0	0.000000	0.000000	1.399804
8	6	0	0.000000	0.000000	-1.399804
9	6	0	0.000000	-1.218634	-0.721788
10	6	0	0.000000	-1.218634	0.721788
11	6	0	0.000000	-2.457570	1.400029
12	1	0	0.000000	-2.457932	2.485080
13	6	0	0.000000	-3.656098	0.722793
14	6	0	0.000000	-3.656098	-0.722793
15	6	0	0.000000	-2.457570	-1.400029
16	1	0	0.000000	0.000000	2.484768
17	1	0	0.000000	2.457932	2.485080
18	1	0	0.000000	2.457932	-2.485080
19	1	0	0.000000	0.000000	-2.484768
20	1	0	0.000000	-2.457932	-2.485080
21	6	0	0.000000	-4.920731	-1.404935
22	1	0	0.000000	-4.919032	-2.489215
23	6	0	0.000000	-4.920731	1.404935
24	1	0	0.000000	-4.919032	2.489215
25	6	0	0.000000	-6.084919	-0.716811
26	1	0	0.000000	-7.030936	-1.244822
27	6	0	0.000000	-6.084919	0.716811
28	1	0	0.000000	-7.030936	1.244822
29	6	0	0.000000	4.920731	-1.404935
30	1	0	0.000000	4.919032	-2.489215
31	6	0	0.000000	6.084919	-0.716811
32	1	0	0.000000	7.030936	-1.244822
33	6	0	0.000000	4.920731	1.404935
34	1	0	0.000000	4.919032	2.489215
35	6	0	0.000000	6.084919	0.716811
36	1	0	0.000000	7.030936	1.244822

T1 coordinates:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	3.697236	-0.709633
2	6	0	0.000000	2.448804	-1.396418
3	6	0	0.000000	1.242468	-0.727628
4	6	0	0.000000	1.242468	0.727628
5	6	0	0.000000	2.448804	1.396418
6	6	0	0.000000	3.697236	0.709633
7	6	0	0.000000	0.000000	-1.405894
8	6	0	0.000000	0.000000	1.405894
9	6	0	0.000000	-1.242468	0.727628
10	6	0	0.000000	-1.242468	-0.727628
11	6	0	0.000000	-2.448804	-1.396418
12	1	0	0.000000	-2.454245	-2.481395
13	6	0	0.000000	-3.697236	-0.709633
14	6	0	0.000000	-3.697236	0.709633
15	6	0	0.000000	-2.448804	1.396418
16	1	0	0.000000	0.000000	-2.490424
17	1	0	0.000000	2.454245	-2.481395
18	1	0	0.000000	2.454245	2.481395
19	1	0	0.000000	0.000000	2.490424
20	1	0	0.000000	-2.454245	2.481395
21	6	0	0.000000	-4.926735	1.391586
22	1	0	0.000000	-4.925091	2.475969
23	6	0	0.000000	-4.926735	-1.391586
24	1	0	0.000000	-4.925091	-2.475969
25	6	0	0.000000	-6.117598	0.700486
26	1	0	0.000000	-7.057239	1.239478
27	6	0	0.000000	-6.117598	-0.700486
28	1	0	0.000000	-7.057239	-1.239478
29	6	0	0.000000	4.926735	1.391586
30	1	0	0.000000	4.925091	2.475969
31	6	0	0.000000	6.117598	0.700486
32	1	0	0.000000	7.057239	1.239478
33	6	0	0.000000	4.926735	-1.391586
34	1	0	0.000000	4.925091	-2.475969
35	6	0	0.000000	6.117598	-0.700486
36	1	0	0.000000	7.057239	-1.239478
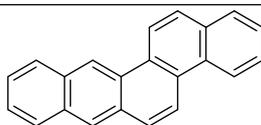
	S0					T1			
	E = -846.5213936 a.u.					E = -846.4460853 a.u.			

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.464430	-1.662725	0.000000
2	6	0	-0.461898	-0.615910	0.000000
3	6	0	0.000000	0.768414	0.000000
4	6	0	1.406015	1.029702	0.000000
5	6	0	2.313688	-0.078714	0.000000
6	6	0	1.868115	-1.349983	0.000000
7	6	0	-0.862545	1.855837	0.000000
8	6	0	1.872954	2.335282	0.000000
9	6	0	1.002858	3.426843	0.000000
10	6	0	-0.400343	3.176373	0.000000
11	6	0	-1.292749	4.287642	0.000000
12	1	0	-2.360184	4.096758	0.000000

T1 coordinates:

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.534897	-1.677886	0.000000
2	6	0	-0.427946	-0.615799	0.000000
3	6	0	0.000000	0.736818	0.000000
4	6	0	1.390220	1.026087	0.000000
5	6	0	2.302291	-0.021164	0.000000
6	6	0	1.884787	-1.346708	0.000000
7	6	0	-0.905378	1.841143	0.000000
8	6	0	1.834931	2.393299	0.000000
9	6	0	0.930699	3.489846	0.000000
10	6	0	-0.471979	3.206840	0.000000
11	6	0	-1.368673	4.262142	0.000000
12	1	0	-2.432727	4.053480	0.000000

S60

13	6	0	-0.819251	5.562990	0.000000
14	6	0	0.580039	5.811034	0.000000
15	6	0	1.462248	4.775630	0.000000
16	1	0	-1.934043	1.708077	0.000000
17	1	0	3.377906	0.128123	0.000000
18	1	0	2.591650	-2.152162	0.000000
19	1	0	2.943711	2.511219	0.000000
20	1	0	-1.507724	6.399460	0.000000
21	1	0	0.939225	6.833135	0.000000
22	1	0	2.530670	4.960418	0.000000
23	6	0	-1.852747	-0.927134	0.000000
24	1	0	-2.580830	-0.128716	0.000000
25	6	0	0.006302	-3.033476	0.000000
26	6	0	-1.383691	-3.298859	0.000000
27	6	0	-2.294749	-2.207836	0.000000
28	1	0	-3.358251	-2.418475	0.000000
29	6	0	0.885355	-4.141999	0.000000
30	1	0	1.954843	-3.987636	0.000000
31	6	0	-1.846986	-4.632566	0.000000
32	1	0	-2.916789	-4.809518	0.000000
33	6	0	-0.969508	-5.682218	0.000000
34	1	0	-1.333786	-6.702362	0.000000
35	6	0	0.412812	-5.428606	0.000000
36	1	0	1.111502	-6.256647	0.000000

13	6	0	-0.921683	5.600321	0.000000
14	6	0	0.423066	5.871730	0.000000
15	6	0	1.352233	4.813765	0.000000
16	1	0	-1.972153	1.670627	0.000000
17	1	0	3.362874	0.203729	0.000000
18	1	0	2.638760	-2.120766	0.000000
19	1	0	2.901110	2.588681	0.000000
20	1	0	-1.645041	6.406314	0.000000
21	1	0	0.776745	6.895427	0.000000
22	1	0	2.414571	5.030366	0.000000
23	6	0	-1.821472	-0.963578	0.000000
24	1	0	-2.565169	-0.180058	0.000000
25	6	0	0.078773	-3.065563	0.000000
26	6	0	-1.304725	-3.338461	0.000000
27	6	0	-2.235769	-2.245826	0.000000
28	1	0	-3.295374	-2.475585	0.000000
29	6	0	0.963051	-4.159621	0.000000
30	1	0	2.031526	-3.994753	0.000000
31	6	0	-1.759155	-4.667843	0.000000
32	1	0	-2.827673	-4.852610	0.000000
33	6	0	-0.872854	-5.718048	0.000000
34	1	0	-1.233204	-6.739523	0.000000
35	6	0	0.500985	-5.456194	0.000000
36	1	0	1.207954	-6.277130	0.000000
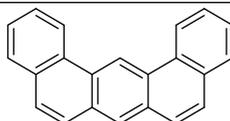
	S_0						T_1				
E = -846.526744 a.u.						E = -846.4343809 a.u.					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.699295	0.284078	1	6	0	0.000000	3.731278	0.300998
2	6	0	0.000000	2.506054	-0.470565	2	6	0	0.000000	2.507433	-0.447963
3	6	0	0.000000	1.223446	0.229196	3	6	0	0.000000	1.265258	0.242800
4	6	0	0.000000	1.216288	1.650388	4	6	0	0.000000	1.261402	1.650646
5	6	0	0.000000	2.460494	2.370740	5	6	0	0.000000	2.468246	2.357445
6	6	0	0.000000	3.638705	1.721551	6	6	0	0.000000	3.682518	1.698914
7	6	0	0.000000	0.000000	-0.436512	7	6	0	0.000000	0.000000	-0.439722
8	6	0	0.000000	0.000000	2.323492	8	6	0	0.000000	0.000000	2.344142
9	6	0	0.000000	-1.216288	1.650388	9	6	0	0.000000	-1.261402	1.650646
10	6	0	0.000000	-1.223446	0.229196	10	6	0	0.000000	-1.265258	0.242800
11	6	0	0.000000	-2.506054	-0.470565	11	6	0	0.000000	-2.507433	-0.447963
12	6	0	0.000000	-3.699295	0.284078	12	6	0	0.000000	-3.731278	0.300998
13	6	0	0.000000	-3.638705	1.721551	13	6	0	0.000000	-3.682518	1.698914
14	6	0	0.000000	-2.460494	2.370740	14	6	0	0.000000	-2.468246	2.357445
15	1	0	0.000000	0.000000	-1.515419	15	1	0	0.000000	0.000000	-1.516307
16	1	0	0.000000	2.425465	3.454301	16	1	0	0.000000	2.440809	3.441305
17	1	0	0.000000	4.572452	2.272519	17	1	0	0.000000	4.609184	2.260904
18	1	0	0.000000	0.000000	3.408608	18	1	0	0.000000	0.000000	3.427604
19	1	0	0.000000	-4.572452	2.272519	19	1	0	0.000000	-4.609184	2.260904
20	1	0	0.000000	-2.425465	3.454301	20	1	0	0.000000	-2.440809	3.441305
21	6	0	0.000000	2.612455	-1.872647	21	6	0	0.000000	2.608087	-1.870133
22	1	0	0.000000	1.720480	-2.484188	22	1	0	0.000000	1.711006	-2.473055
23	6	0	0.000000	4.941174	-0.374703	23	6	0	0.000000	4.973844	-0.391644
24	6	0	0.000000	5.016122	-1.746395	24	6	0	0.000000	5.022269	-1.750654
25	6	0	0.000000	3.837313	-2.499696	25	6	0	0.000000	3.816802	-2.497749
26	1	0	0.000000	3.886850	-3.581951	26	1	0	0.000000	3.860903	-3.580295
27	1	0	0.000000	5.979214	-2.242207	27	1	0	0.000000	5.974463	-2.266868
28	1	0	0.000000	5.846424	0.222313	28	1	0	0.000000	5.886950	0.193141
29	6	0	0.000000	-2.612455	-1.872647	29	6	0	0.000000	-2.608087	-1.870133
30	1	0	0.000000	-1.720480	-2.484188	30	1	0	0.000000	-1.711006	-2.473055
31	6	0	0.000000	-4.941174	-0.374703	31	6	0	0.000000	-4.973844	-0.391644
32	1	0	0.000000	-5.846424	0.222313	32	1	0	0.000000	-5.886950	0.193141
33	6	0	0.000000	-5.016122	-1.746395	33	6	0	0.000000	-5.022269	-1.750654

Center Number	Atomic Number	Atomic Type	X	Y	Z		Center Number	Atomic Number	Atomic Type	X	Y	Z
34	1	0	0.000000	-5.979214	-2.242207		34	1	0	0.000000	-5.974463	-2.266868
35	6	0	0.000000	-3.837313	-2.499696		35	6	0	0.000000	-3.816802	-2.497749
36	1	0	0.000000	-3.886850	-3.581951		36	1	0	0.000000	-3.860903	-3.580295
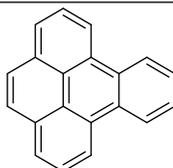
	S₀						T₁					
	E = -769.1454581 a.u.						E = -769.0546043 a.u.					

Center Number	Atomic Number	Atomic Type	X	Y	Z		Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	3.510567	-0.915357		1	6	0	0.000000	-3.547116	-0.902042
2	6	0	0.000000	2.812117	-2.104462		2	6	0	0.000000	-2.858615	-2.098874
3	6	0	0.000000	1.415313	-2.099445		3	6	0	0.000000	-1.421751	-2.112509
4	6	0	0.000000	0.717555	-0.865486		4	6	0	0.000000	-0.715314	-0.852846
5	6	0	0.000000	1.440188	0.351660		5	6	0	0.000000	-1.427731	0.352069
6	6	0	0.000000	2.831619	0.296451		6	6	0	0.000000	-2.871706	0.302735
7	6	0	0.000000	0.673262	-3.327931		7	6	0	0.000000	-0.715679	-3.289700
8	6	0	0.000000	-0.717555	-0.865486		8	6	0	0.000000	0.715314	-0.852846
9	6	0	0.000000	-1.415313	-2.099445		9	6	0	0.000000	1.421751	-2.112509
10	6	0	0.000000	-0.673262	-3.327931		10	6	0	0.000000	0.715679	-3.289700
11	6	0	0.000000	-2.812117	-2.104462		11	6	0	0.000000	2.858615	-2.098874
12	1	0	0.000000	-3.338028	-3.052265		12	1	0	0.000000	3.386748	-3.044604
13	6	0	0.000000	-3.510567	-0.915357		13	6	0	0.000000	3.547116	-0.902042
14	6	0	0.000000	-2.831619	0.296451		14	6	0	0.000000	2.871706	0.302735
15	6	0	0.000000	-1.440188	0.351660		15	6	0	0.000000	1.427731	0.352069
16	6	0	0.000000	-0.703878	1.620501		16	6	0	0.000000	0.713339	1.590672
17	6	0	0.000000	0.703878	1.620501		17	6	0	0.000000	-0.713339	1.590672
18	1	0	0.000000	1.226340	-4.260307		18	1	0	0.000000	-1.248248	-4.233248
19	1	0	0.000000	4.593834	-0.920726		19	1	0	0.000000	-4.630783	-0.904338
20	1	0	0.000000	3.338028	-3.052265		20	1	0	0.000000	-3.386748	-3.044604
21	1	0	0.000000	3.414418	1.206152		21	1	0	0.000000	-3.443806	1.217547
22	1	0	0.000000	-1.226340	-4.260307		22	1	0	0.000000	1.248248	-4.233248
23	1	0	0.000000	-4.593834	-0.920726		23	1	0	0.000000	4.630783	-0.904338
24	1	0	0.000000	-3.414418	1.206152		24	1	0	0.000000	3.443806	1.217547
25	6	0	0.000000	-1.376951	2.854777		25	6	0	0.000000	1.385203	2.841878
26	1	0	0.000000	-2.457071	2.878647		26	1	0	0.000000	2.464847	2.869575
27	6	0	0.000000	1.376951	2.854777		27	6	0	0.000000	-1.385203	2.841878
28	1	0	0.000000	2.457071	2.878647		28	1	0	0.000000	-2.464847	2.869575
29	6	0	0.000000	0.697504	4.049935		29	6	0	0.000000	-0.704380	4.024113
30	1	0	0.000000	1.244801	4.984650		30	1	0	0.000000	-1.246333	4.962088
31	6	0	0.000000	-0.697504	4.049935		31	6	0	0.000000	0.704380	4.024113
32	1	0	0.000000	-1.244801	4.984650		32	1	0	0.000000	1.246333	4.962088

	S₀						T₁					
	E = -308.252107 a.u.						E = -308.206372 a.u.					

Center Number	Atomic Number	Atomic Type	X	Y	Z		Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	1.437733	-0.620635		1	6	0	0.000000	1.456203	-0.630279
2	6	0	0.000000	0.709259	0.518543		2	6	0	0.000000	0.726552	0.557170
3	6	0	0.000000	-0.709259	0.518543		3	6	0	0.000000	-0.726552	0.557170
4	6	0	0.000000	-1.437733	-0.620635		4	6	0	0.000000	-1.456203	-0.630279
5	6	0	0.000000	-0.684667	-1.836916		5	6	0	0.000000	-0.710968	-1.796279
6	6	0	0.000000	0.684667	-1.836916		6	6	0	0.000000	0.710968	-1.796279
7	1	0	0.000000	2.520745	-0.640971		7	1	0	0.000000	2.538900	-0.655968
8	1	0	0.000000	-2.520745	-0.640971		8	1	0	0.000000	-2.538900	-0.655968
9	1	0	0.000000	-1.215322	-2.781576		9	1	0	0.000000	-1.220749	-2.752418

10	1	0	0.000000	1.215322	-2.781576
11	6	0	0.000000	-0.670951	2.039732
12	1	0	0.000000	-1.420166	2.818205
13	6	0	0.000000	0.670951	2.039732
14	1	0	0.000000	1.420166	2.818205

10	1	0	0.000000	1.220749	-2.752418
11	6	0	0.000000	-0.739453	1.980111
12	1	0	0.000000	-1.501377	2.744043
13	6	0	0.000000	0.739453	1.980111
14	1	0	0.000000	1.501377	2.744043
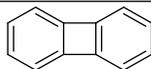
S_0		T_1	
E = -461.8676973 a.u.		E = -461.7897602 a.u.	

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X Y Z			Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X Y Z		
1	6	0	0.000000	1.437048	1.906717	1	6	0	0.000000	1.464778	1.908593
2	6	0	0.000000	0.707598	0.754054	2	6	0	0.000000	0.736927	0.711990
3	6	0	0.000000	-0.707598	0.754054	3	6	0	0.000000	-0.736927	0.711990
4	6	0	0.000000	-1.437048	1.906717	4	6	0	0.000000	-1.464778	1.908593
5	6	0	0.000000	-0.690447	3.107692	5	6	0	0.000000	-0.722209	3.064171
6	6	0	0.000000	0.690447	3.107692	6	6	0	0.000000	0.722209	3.064171
7	1	0	0.000000	2.519787	1.926560	7	1	0	0.000000	2.547533	1.938710
8	1	0	0.000000	-2.519787	1.926560	8	1	0	0.000000	-2.547533	1.938710
9	1	0	0.000000	-1.216860	4.054740	9	1	0	0.000000	-1.226618	4.022934
10	1	0	0.000000	1.216860	4.054740	10	1	0	0.000000	1.226618	4.022934
11	6	0	0.000000	-0.707598	-0.754054	11	6	0	0.000000	-0.736927	-0.711990
12	6	0	0.000000	0.707598	-0.754054	12	6	0	0.000000	0.736927	-0.711990
13	6	0	0.000000	-1.437048	-1.906717	13	6	0	0.000000	-1.464778	-1.908593
14	1	0	0.000000	-2.519787	-1.926560	14	1	0	0.000000	-2.547533	-1.938710
15	6	0	0.000000	1.437048	-1.906717	15	6	0	0.000000	1.464778	-1.908593
16	1	0	0.000000	2.519787	-1.926560	16	1	0	0.000000	2.547533	-1.938710
17	6	0	0.000000	0.690447	-3.107692	17	6	0	0.000000	0.722209	-3.064171
18	1	0	0.000000	1.216860	-4.054740	18	1	0	0.000000	1.226618	-4.022934
19	6	0	0.000000	-0.690447	-3.107692	19	6	0	0.000000	-0.722209	-3.064171
20	1	0	0.000000	-1.216860	-4.054740	20	1	0	0.000000	-1.226618	-4.022934
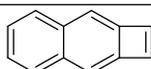
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1	6	0	0.000000	0.697400	-3.035625	1	6	0	0.000000	0.708866	-3.013002
2	6	0	0.000000	1.384700	-1.838472	2	6	0	0.000000	1.394166	-1.835270
3	6	0	0.000000	0.710721	-0.611224	3	6	0	0.000000	0.722953	-0.581363
4	6	0	0.000000	-0.710721	-0.611224	4	6	0	0.000000	-0.722953	-0.581363
5	6	0	0.000000	-1.384700	-1.838472	5	6	0	0.000000	-1.394166	-1.835270
6	6	0	0.000000	-0.697400	-3.035625	6	6	0	0.000000	-0.708866	-3.013002
7	1	0	0.000000	2.533670	0.621509	7	1	0	0.000000	2.540480	0.599340
8	1	0	0.000000	1.240631	-3.972920	8	1	0	0.000000	1.244268	-3.954652
9	1	0	0.000000	2.469387	-1.836917	9	1	0	0.000000	2.478408	-1.834252
10	6	0	0.000000	1.450020	0.643772	10	6	0	0.000000	1.457158	0.625662
11	6	0	0.000000	-1.450020	0.643772	11	6	0	0.000000	-1.457158	0.625662
12	1	0	0.000000	-2.469387	-1.836917	12	1	0	0.000000	-2.478408	-1.834252
13	1	0	0.000000	-1.240631	-3.972920	13	1	0	0.000000	-1.244268	-3.954652
14	6	0	0.000000	-0.723167	1.765053	14	6	0	0.000000	-0.733450	1.795220
15	6	0	0.000000	0.723167	1.765053	15	6	0	0.000000	0.733450	1.795220
16	1	0	0.000000	-2.533670	0.621509	16	1	0	0.000000	-2.540480	0.599340
17	6	0	0.000000	-0.674150	3.266606	17	6	0	0.000000	-0.752130	3.211422
18	1	0	0.000000	-1.420820	4.047673	18	1	0	0.000000	-1.515614	3.973541
19	6	0	0.000000	0.674150	3.266606	19	6	0	0.000000	0.752130	3.211422
20	1	0	0.000000	1.420820	4.047673	20	1	0	0.000000	1.515614	3.973541
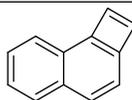
	S₀						T₁				

E = -461.83291 a.u.

E = -461.8039873 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
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1	6	0	-2.685173	1.383964	0.000000
2	6	0	-2.406203	0.054399	0.000000
3	6	0	-1.059594	-0.421214	0.000000
4	6	0	0.000000	0.562701	0.000000
5	6	0	-0.335226	1.952196	0.000000
6	6	0	-1.633650	2.346949	0.000000
7	1	0	-1.591553	-2.491389	0.000000
8	1	0	-3.714012	1.723448	0.000000
9	1	0	-3.209387	-0.674582	0.000000
10	6	0	-0.765135	-1.789416	0.000000
11	6	0	1.274595	0.041868	0.000000
12	1	0	0.466106	2.682030	0.000000
13	1	0	-1.881502	3.401838	0.000000
14	6	0	1.539487	-1.321413	0.000000
15	6	0	0.549258	-2.271882	0.000000
16	1	0	0.749648	-3.336274	0.000000
17	6	0	3.041447	-1.001804	0.000000
18	1	0	3.946072	-1.592081	0.000000
19	6	0	2.785372	0.311897	0.000000
20	1	0	3.403563	1.197540	0.000000

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.667986	1.417781	0.000000
2	6	0	-2.368986	0.069768	0.000000
3	6	0	-1.041830	-0.378993	0.000000
4	6	0	0.000000	0.595704	0.000000
5	6	0	-0.324248	1.961482	0.000000
6	6	0	-1.640921	2.367641	0.000000
7	1	0	-1.587560	-2.476648	0.000000
8	1	0	-3.701782	1.741321	0.000000
9	1	0	-3.170122	-0.661197	0.000000
10	6	0	-0.743326	-1.796538	0.000000
11	6	0	1.313242	0.063838	0.000000
12	1	0	0.474823	2.693578	0.000000
13	1	0	-1.882378	3.423685	0.000000
14	6	0	1.569517	-1.363052	0.000000
15	6	0	0.537451	-2.300035	0.000000
16	1	0	0.716216	-3.368323	0.000000
17	6	0	2.981295	-1.100823	0.000000
18	1	0	3.875652	-1.704417	0.000000
19	6	0	2.710302	0.320891	0.000000
20	1	0	3.328095	1.206017	0.000000
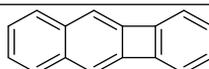
	S₀						T₁				

E = -615.46347 a.u.

E = -615.3460238 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	-0.700283	-4.300120
2	6	0	0.000000	-1.387251	-3.108985
3	6	0	0.000000	-0.712168	-1.875223
4	6	0	0.000000	0.712168	-1.875223
5	6	0	0.000000	1.387251	-3.108985
6	6	0	0.000000	0.700283	-4.300120
7	1	0	0.000000	-2.530561	-0.654273
8	1	0	0.000000	-1.241336	-5.238635
9	1	0	0.000000	-2.471718	-3.107644
10	6	0	0.000000	-1.447113	-0.632276
11	6	0	0.000000	1.447113	-0.632276
12	1	0	0.000000	2.471718	-3.107644
13	1	0	0.000000	1.241336	-5.238635
14	6	0	0.000000	0.721726	0.499341
15	6	0	0.000000	-0.721726	0.499341
16	1	0	0.000000	2.530561	-0.654273
17	6	0	0.000000	0.706353	1.998078
18	6	0	0.000000	-0.706353	1.998078
19	6	0	0.000000	1.437502	3.156458
20	1	0	0.000000	2.520122	3.175606
21	6	0	0.000000	-1.437502	3.156458
22	1	0	0.000000	-2.520122	3.175606
23	6	0	0.000000	-0.693344	4.350425
24	1	0	0.000000	-1.217378	5.298760
25	6	0	0.000000	0.693344	4.350425
26	1	0	0.000000	1.217378	5.298760

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	-0.699647	-4.286949
2	6	0	0.000000	-1.390274	-3.093050
3	6	0	0.000000	-0.728609	-1.850706
4	6	0	0.000000	0.728609	-1.850706
5	6	0	0.000000	1.390274	-3.093050
6	6	0	0.000000	0.699647	-4.286949
7	1	0	0.000000	-2.555744	-0.647387
8	1	0	0.000000	-1.241127	-5.225121
9	1	0	0.000000	-2.474200	-3.095092
10	6	0	0.000000	-1.474866	-0.630685
11	6	0	0.000000	1.474866	-0.630685
12	1	0	0.000000	2.474200	-3.095092
13	1	0	0.000000	1.241127	-5.225121
14	6	0	0.000000	0.721715	0.527245
15	6	0	0.000000	-0.721715	0.527245
16	1	0	0.000000	2.555744	-0.647387
17	6	0	0.000000	0.723577	1.970511
18	6	0	0.000000	-0.723577	1.970511
19	6	0	0.000000	1.471000	3.134236
20	1	0	0.000000	2.551083	3.155760
21	6	0	0.000000	-1.471000	3.134236
22	1	0	0.000000	-2.551083	3.155760
23	6	0	0.000000	-0.697192	4.318730
24	1	0	0.000000	-1.205488	5.275851
25	6	0	0.000000	0.697192	4.318730
26	1	0	0.000000	1.205488	5.275851

	S₀		
	E = -615.4528847 a.u.		

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Structure 1 (dibenzo — first molecule)

S_0 — E = -615.4528847 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	2.602357	-3.157937	0.000000
2	6	0	1.251872	-3.341591	0.000000
3	6	0	0.359919	-2.234021	0.000000
4	6	0	0.926035	-0.914710	0.000000
5	6	0	2.338743	-0.758017	0.000000
6	6	0	3.152554	-1.850254	0.000000
7	1	0	-1.417706	-3.435512	0.000000
8	1	0	3.266489	-4.013767	0.000000
9	1	0	0.835411	-4.342805	0.000000
10	6	0	-1.040230	-2.419110	0.000000
11	6	0	0.000000	0.122824	0.000000
12	1	0	2.754222	0.242625	0.000000
13	1	0	4.228861	-1.726514	0.000000
14	6	0	-1.372375	-0.089939	0.000000
15	6	0	-1.932014	-1.358192	0.000000
16	1	0	-3.001109	-1.529111	0.000000
17	6	0	-1.616057	1.402727	0.000000
18	6	0	-0.213995	1.618650	0.000000
19	6	0	-2.511200	2.426096	0.000000
20	1	0	-3.584306	2.281094	0.000000
21	6	0	0.330303	2.865432	0.000000
22	1	0	1.396794	3.052806	0.000000
23	6	0	-0.594501	3.942936	0.000000
24	1	0	-0.217178	4.958520	0.000000
25	6	0	-1.954814	3.732705	0.000000
26	1	0	-2.621059	4.587075	0.000000

T_1 — E = -615.3946886 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	3.136207	-2.635094	0.000000
2	6	0	1.800011	-3.032360	0.000000
3	6	0	0.769425	-2.100852	0.000000
4	6	0	1.110766	-0.711301	0.000000
5	6	0	2.454624	-0.329924	0.000000
6	6	0	3.461147	-1.286779	0.000000
7	1	0	-0.800799	-3.608174	0.000000
8	1	0	3.919401	-3.383275	0.000000
9	1	0	1.555821	-4.088977	0.000000
10	6	0	-0.625808	-2.538722	0.000000
11	6	0	0.000000	0.170246	0.000000
12	1	0	2.705993	0.724139	0.000000
13	1	0	4.499376	-0.977659	0.000000
14	6	0	-1.399197	-0.320040	0.000000
15	6	0	-1.701816	-1.668841	0.000000
16	1	0	-2.717440	-2.045693	0.000000
17	6	0	-1.850872	1.051824	0.000000
18	6	0	-0.479057	1.513716	0.000000
19	6	0	-2.920998	1.934946	0.000000
20	1	0	-3.953828	1.609402	0.000000
21	6	0	-0.172162	2.878222	0.000000
22	1	0	0.843140	3.254327	0.000000
23	6	0	-1.251863	3.739489	0.000000
24	1	0	-1.076188	4.808800	0.000000
25	6	0	-2.595032	3.283077	0.000000
26	1	0	-3.387725	4.021474	0.000000

Structure 2 (second molecule)

S_0 — E = -615.4405653 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	0.707354	-4.241016
2	6	0	0.000000	1.395773	-3.062200
3	6	0	0.000000	0.710208	-1.820127
4	6	0	0.000000	-0.710208	-1.820127
5	6	0	0.000000	-1.395773	-3.062200
6	6	0	0.000000	-0.707354	-4.241016
7	6	0	0.000000	1.388653	-0.584758
8	6	0	0.000000	-1.388653	-0.584758
9	6	0	0.000000	-0.722214	0.618497
10	6	0	0.000000	0.722214	0.618497
11	6	0	0.000000	1.457537	1.882536
12	1	0	0.000000	2.541186	1.862261
13	6	0	0.000000	0.729074	2.998456
14	6	0	0.000000	-0.729074	2.998456
15	6	0	0.000000	-1.457537	1.882536
16	1	0	0.000000	2.474132	-0.587846
17	1	0	0.000000	1.241539	-5.183594
18	1	0	0.000000	2.480254	-3.058523
19	1	0	0.000000	-2.480254	-3.058523
20	1	0	0.000000	-1.241539	-5.183594
21	1	0	0.000000	-2.474132	-0.587846
22	1	0	0.000000	-2.541186	1.862261

T_1 — E = -615.3506129 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	-0.681513	-4.301508
2	6	0	0.000000	-1.389894	-3.068850
3	6	0	0.000000	-0.720140	-1.854302
4	6	0	0.000000	0.720140	-1.854302
5	6	0	0.000000	1.389894	-3.068850
6	6	0	0.000000	0.681513	-4.301508
7	6	0	0.000000	-1.396023	-0.606341
8	6	0	0.000000	1.396023	-0.606341
9	6	0	0.000000	0.702143	0.657913
10	6	0	0.000000	-0.702143	0.657913
11	6	0	0.000000	-1.433613	1.882665
12	1	0	0.000000	-2.517327	1.862607
13	6	0	0.000000	-0.705882	3.028248
14	6	0	0.000000	0.705882	3.028248
15	6	0	0.000000	1.433613	1.882665
16	1	0	0.000000	-2.480153	-0.600702
17	1	0	0.000000	-1.233909	-5.233042
18	1	0	0.000000	-2.473938	-3.075908
19	1	0	0.000000	2.473938	-3.075908
20	1	0	0.000000	1.233909	-5.233042
21	1	0	0.000000	2.480153	-0.600702
22	1	0	0.000000	2.517327	1.862607

Center Number	Atomic Number	Atomic Type	X	Y	Z
23	6	0	0.000000	-0.675895	4.491036
24	1	0	0.000000	-1.421587	5.273152
25	6	0	0.000000	0.675895	4.491036
26	1	0	0.000000	1.421587	5.273152

Center Number	Atomic Number	Atomic Type	X	Y	Z
23	6	0	0.000000	0.671347	4.548986
24	1	0	0.000000	1.421569	5.326186
25	6	0	0.000000	-0.671347	4.548986
26	1	0	0.000000	-1.421569	5.326186

	S_0
	E = -615.4115848 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-1.297480	-4.000845	0.000000
2	6	0	-0.105072	-3.358554	0.000000
3	6	0	-0.035135	-1.926735	0.000000
4	6	0	-1.266984	-1.178781	0.000000
5	6	0	-2.504365	-1.904713	0.000000
6	6	0	-2.520124	-3.258733	0.000000
7	6	0	1.172988	-1.252821	0.000000
8	6	0	-1.224273	0.202026	0.000000
9	6	0	0.000000	0.894447	0.000000
10	6	0	1.244891	0.149324	0.000000
11	6	0	2.487837	0.826146	0.000000
12	1	0	3.392091	0.228287	0.000000
13	6	0	2.578294	2.210073	0.000000
14	6	0	1.377575	2.900500	0.000000
15	6	0	0.152722	2.275009	0.000000
16	1	0	2.096060	-1.823664	0.000000
17	1	0	-1.334754	-5.083526	0.000000
18	1	0	0.823540	-3.918475	0.000000
19	1	0	-3.430951	-1.341567	0.000000
20	1	0	-3.462936	-3.792594	0.000000
21	1	0	-2.150402	0.766205	0.000000
22	1	0	3.541874	2.704329	0.000000
23	6	0	0.656879	4.263443	0.000000
24	1	0	0.975951	5.295286	0.000000
25	6	0	-0.533449	3.654385	0.000000
26	1	0	-1.556301	4.000705	0.000000

	T_1
	E = -615.3923524 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	1.477896	-3.944452	0.000000
2	6	0	0.253736	-3.333619	0.000000
3	6	0	0.145975	-1.922900	0.000000
4	6	0	1.335294	-1.142394	0.000000
5	6	0	2.587974	-1.805113	0.000000
6	6	0	2.658650	-3.170355	0.000000
7	6	0	-1.107638	-1.267061	0.000000
8	6	0	1.229270	0.263391	0.000000
9	6	0	0.000000	0.894271	0.000000
10	6	0	-1.217582	0.102421	0.000000
11	6	0	-2.521525	0.743120	0.000000
12	1	0	-3.386968	0.090586	0.000000
13	6	0	-2.696964	2.112085	0.000000
14	6	0	-1.542342	2.883789	0.000000
15	6	0	-0.212387	2.292851	0.000000
16	1	0	-2.007840	-1.873328	0.000000
17	1	0	1.546086	-5.025616	0.000000
18	1	0	-0.654508	-3.926084	0.000000
19	1	0	3.493411	-1.208458	0.000000
20	1	0	3.622729	-3.664574	0.000000
21	1	0	2.135526	0.859102	0.000000
22	1	0	-3.690688	2.543395	0.000000
23	6	0	-0.935402	4.192652	0.000000
24	1	0	-1.303747	5.207211	0.000000
25	6	0	0.358769	3.601483	0.000000
26	1	0	1.363662	3.996748	0.000000

	S_0
	E = -615.440046 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	2.795962	-2.954153	0.000000
2	6	0	1.452086	-3.205453	0.000000
3	6	0	0.511372	-2.150431	0.000000
4	6	0	0.962296	-0.805788	0.000000
5	6	0	2.361107	-0.583187	0.000000
6	6	0	3.251833	-1.623283	0.000000
7	6	0	-0.883818	-2.419926	0.000000
8	6	0	0.000000	0.267334	0.000000
9	6	0	-1.371483	-0.044745	0.000000
10	6	0	-1.783794	-1.405122	0.000000
11	6	0	-2.383242	0.994494	0.000000
12	1	0	-3.429803	0.712802	0.000000
13	6	0	-1.947032	2.260240	0.000000
14	6	0	-0.550364	2.584728	0.000000
15	6	0	0.417407	1.657561	0.000000

	T_1
	E = -615.3860517 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	2.932572	-2.815493	0.000000
2	6	0	1.591050	-3.117980	0.000000
3	6	0	0.619097	-2.104921	0.000000
4	6	0	1.014545	-0.749051	0.000000
5	6	0	2.393032	-0.469984	0.000000
6	6	0	3.332729	-1.476582	0.000000
7	6	0	-0.779350	-2.439493	0.000000
8	6	0	0.000000	0.303674	0.000000
9	6	0	-1.394638	-0.085702	0.000000
10	6	0	-1.725577	-1.480941	0.000000
11	6	0	-2.434128	0.859655	0.000000
12	1	0	-3.464362	0.523474	0.000000
13	6	0	-2.075804	2.188467	0.000000
14	6	0	-0.673073	2.587854	0.000000
15	6	0	0.351737	1.660012	0.000000

16	1	0	-1.215806	-3.451917	0.000000
17	1	0	3.507336	-3.771086	0.000000
18	1	0	1.083501	-4.225366	0.000000
19	1	0	2.747455	0.426291	0.000000
20	1	0	4.315950	-1.419333	0.000000
21	1	0	-2.846935	-1.618963	0.000000
22	1	0	1.465208	1.921283	0.000000
23	6	0	-2.246276	3.738469	0.000000
24	1	0	-3.151356	4.328522	0.000000
25	6	0	-0.934762	4.043446	0.000000
26	1	0	-0.383298	4.972660	0.000000

16	1	0	-1.056698	-3.487462	0.000000
17	1	0	3.672584	-3.606480	0.000000
18	1	0	1.263899	-4.151815	0.000000
19	1	0	2.739476	0.554005	0.000000
20	1	0	4.386733	-1.226096	0.000000
21	1	0	-2.775955	-1.749409	0.000000
22	1	0	1.386039	1.972836	0.000000
23	6	0	-2.477206	3.551648	0.000000
24	1	0	-3.418539	4.078714	0.000000
25	6	0	-1.044217	3.954769	0.000000
26	1	0	-0.517796	4.896640	0.000000

S_0	T_1
E = -615.4275101 a.u.	E = -615.3921576 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z	Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	3.905243	-1.209253	0.000000	1	6	0	3.844935	-1.343454	0.000000
2	6	0	2.779179	-1.998777	0.000000	2	6	0	2.706892	-2.104658	0.000000
3	6	0	1.494431	-1.432485	0.000000	3	6	0	1.428847	-1.507038	0.000000
4	6	0	1.346167	-0.028720	0.000000	4	6	0	1.312978	-0.092192	0.000000
5	6	0	2.512936	0.753613	0.000000	5	6	0	2.509674	0.662687	0.000000
6	6	0	3.765624	0.180674	0.000000	6	6	0	3.739463	0.057201	0.000000
7	6	0	0.330527	-2.286797	0.000000	7	6	0	0.254783	-2.317279	0.000000
8	6	0	0.000000	0.552390	0.000000	8	6	0	0.000000	0.509061	0.000000
9	6	0	-1.127421	-0.355258	0.000000	9	6	0	-1.129417	-0.341764	0.000000
10	6	0	-0.912438	-1.779918	0.000000	10	6	0	-0.977242	-1.756455	0.000000
11	6	0	-2.361606	0.233018	0.000000	11	6	0	-2.384526	0.302146	0.000000
12	6	0	-2.557121	1.617441	0.000000	12	6	0	-2.519394	1.742269	0.000000
13	6	0	-1.515743	2.494008	0.000000	13	6	0	-1.400833	2.569335	0.000000
14	6	0	-0.223251	1.922881	0.000000	14	6	0	-0.173411	1.940863	0.000000
15	1	0	0.488534	-3.359488	0.000000	15	1	0	0.371031	-3.395098	0.000000
16	1	0	4.890483	-1.659313	0.000000	16	1	0	4.820253	-1.814648	0.000000
17	1	0	2.870274	-3.079387	0.000000	17	1	0	2.771453	-3.187068	0.000000
18	1	0	2.440615	1.832530	0.000000	18	1	0	2.468655	1.742604	0.000000
19	1	0	4.644970	0.813613	0.000000	19	1	0	4.636506	0.664784	0.000000
20	1	0	-1.778499	-2.431295	0.000000	20	1	0	-1.866917	-2.374995	0.000000
21	1	0	-1.638317	3.570015	0.000000	21	1	0	-1.467064	3.650367	0.000000
22	1	0	0.620156	2.599189	0.000000	22	1	0	0.709208	2.563943	0.000000
23	6	0	-4.066476	1.374568	0.000000	23	6	0	-3.944832	1.610218	0.000000
24	1	0	-4.939885	2.010061	0.000000	24	1	0	-4.782083	2.290605	0.000000
25	6	0	-3.878996	0.047204	0.000000	25	6	0	-3.796959	0.157700	0.000000
26	1	0	-4.544665	-0.803451	0.000000	26	1	0	-4.486787	-0.672338	0.000000

S_0	T_1
E = -615.4297379 a.u.	E = -615.3953282 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z	Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.252057	-3.808062	0.000000	1	6	0	-0.255908	-3.815682	0.000000
2	6	0	-0.973591	-3.181251	0.000000	2	6	0	0.967822	-3.199346	0.000000
3	6	0	-1.069785	-1.781207	0.000000	3	6	0	1.070858	-1.792271	0.000000
4	6	0	0.107032	-1.006302	0.000000	4	6	0	-0.108700	-1.009345	0.000000
5	6	0	1.344634	-1.665678	0.000000	5	6	0	-1.354682	-1.671003	0.000000
6	6	0	1.420310	-3.041929	0.000000	6	6	0	-1.428226	-3.040856	0.000000

Center	Atomic	Atomic		Coordinates (Angstroms)	
Number	Number	Type	X	Y	Z
7	6	0	-2.357359	-1.128378	0.000000
8	6	0	0.000000	0.449518	0.000000
9	6	0	-1.308260	1.067953	0.000000
10	6	0	-2.467568	0.211678	0.000000
11	6	0	-1.454126	2.448358	0.000000
12	1	0	-2.457613	2.858397	0.000000
13	6	0	-0.349538	3.325197	0.000000
14	6	0	0.873305	2.726976	0.000000
15	6	0	1.044770	1.334313	0.000000
16	1	0	-3.243975	-1.752352	0.000000
17	1	0	0.311376	-4.889738	0.000000
18	1	0	-1.886093	-3.767124	0.000000
19	1	0	2.257585	-1.086105	0.000000
20	1	0	2.387868	-3.529217	0.000000
21	1	0	-3.444884	0.681329	0.000000
22	1	0	-0.490350	4.398803	0.000000
23	6	0	2.389496	2.890799	0.000000
24	1	0	3.063566	3.734750	0.000000
25	6	0	2.560393	1.562444	0.000000
26	1	0	3.431898	0.924686	0.000000

Center	Atomic	Atomic		Coordinates (Angstroms)	
Number	Number	Type	X	Y	Z
7	6	0	2.339695	-1.143326	0.000000
8	6	0	0.000000	0.425055	0.000000
9	6	0	1.276245	1.036598	0.000000
10	6	0	2.433517	0.212395	0.000000
11	6	0	1.433215	2.469719	0.000000
12	1	0	2.447389	2.852792	0.000000
13	6	0	0.374819	3.347279	0.000000
14	6	0	-0.892267	2.768398	0.000000
15	6	0	-1.084811	1.326953	0.000000
16	1	0	3.234868	-1.754805	0.000000
17	1	0	-0.322789	-4.896896	0.000000
18	1	0	1.878506	-3.787955	0.000000
19	1	0	-2.265082	-1.088376	0.000000
20	1	0	-2.395386	-3.529117	0.000000
21	1	0	3.407338	0.689077	0.000000
22	1	0	0.532456	4.418645	0.000000
23	6	0	-2.306339	2.963200	0.000000
24	1	0	-2.965014	3.817582	0.000000
25	6	0	-2.496304	1.521570	0.000000
26	1	0	-3.365888	0.883031	0.000000

	S_0		T_1		
	E = -615.4187187 a.u.		E = -615.3987842 a.u.		

Center	Atomic	Atomic		Coordinates (Angstroms)	
Number	Number	Type	X	Y	Z
1	6	0	0.000000	-3.558915	-0.738238
2	6	0	0.000000	-2.869154	0.441352
3	6	0	0.000000	-1.454071	0.448139
4	6	0	0.000000	-0.725419	-0.783866
5	6	0	0.000000	-1.485099	-1.975396
6	6	0	0.000000	-2.856082	-1.957863
7	6	0	0.000000	-0.679009	1.612942
8	6	0	0.000000	0.725419	-0.783866
9	6	0	0.000000	1.454071	0.448139
10	6	0	0.000000	0.679009	1.612942
11	6	0	0.000000	2.869154	0.441352
12	1	0	0.000000	3.394092	1.389433
13	6	0	0.000000	3.558915	-0.738238
14	6	0	0.000000	2.856082	-1.957863
15	6	0	0.000000	1.485099	-1.975396
16	1	0	0.000000	-4.642242	-0.738760
17	1	0	0.000000	-3.394092	1.389433
18	1	0	0.000000	-0.984754	-2.933799
19	1	0	0.000000	-3.403365	-2.892736
20	1	0	0.000000	4.642242	-0.738760
21	1	0	0.000000	3.403365	-2.892736
22	1	0	0.000000	0.984754	-2.933799
23	6	0	0.000000	-0.668053	3.160049
24	1	0	0.000000	-1.421946	3.933156
25	6	0	0.000000	0.668053	3.160049
26	1	0	0.000000	1.421946	3.933156

Center	Atomic	Atomic		Coordinates (Angstroms)	
Number	Number	Type	X	Y	Z
1	6	0	0.000000	-3.574004	-0.752823
2	6	0	0.000000	-2.888662	0.440382
3	6	0	0.000000	-1.483169	0.461390
4	6	0	0.000000	-0.743287	-0.758362
5	6	0	0.000000	-1.477706	-1.947752
6	6	0	0.000000	-2.861834	-1.952721
7	6	0	0.000000	-0.718865	1.649449
8	6	0	0.000000	0.743287	-0.758362
9	6	0	0.000000	1.483169	0.461390
10	6	0	0.000000	0.718865	1.649449
11	6	0	0.000000	2.888662	0.440382
12	1	0	0.000000	3.424015	1.382569
13	6	0	0.000000	3.574004	-0.752823
14	6	0	0.000000	2.861834	-1.952721
15	6	0	0.000000	1.477706	-1.947752
16	1	0	0.000000	-4.657213	-0.761524
17	1	0	0.000000	-3.424015	1.382569
18	1	0	0.000000	-0.968556	-2.901340
19	1	0	0.000000	-3.391656	-2.897536
20	1	0	0.000000	4.657213	-0.761524
21	1	0	0.000000	3.391656	-2.897536
22	1	0	0.000000	0.968556	-2.901340
23	6	0	0.000000	-0.719054	3.081425
24	1	0	0.000000	-1.474693	3.851899
25	6	0	0.000000	0.719054	3.081425
26	1	0	0.000000	1.474693	3.851899
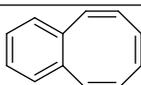
	S_0		T_1		
	E = -463.0622757 a.u.		E = -463.029147 a.u.		

Center	Atomic	Atomic	Coordinates (Angstroms)	Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z		Number	Number	Type	X	Y	Z
1	6	0	0.000000	0.688422	3.043396		1	6	0	0.000000	0.700455	3.033827
2	6	0	0.000000	-0.688422	3.043396		2	6	0	0.000000	-0.700455	3.033827
3	6	0	0.000000	-1.353640	1.824337		3	6	0	0.000000	-1.362507	1.836564
4	6	0	0.000000	-0.707932	0.584950		4	6	0	0.000000	-0.718494	0.566621
5	6	0	0.000000	0.707932	0.584950		5	6	0	0.000000	0.718494	0.566621
6	6	0	0.000000	1.353640	1.824337		6	6	0	0.000000	1.362507	1.836564
7	1	0	0.000000	1.250751	3.968971		7	1	0	0.000000	1.255513	3.963700
8	1	0	0.000000	-1.250751	3.968971		8	1	0	0.000000	-1.255513	3.963700
9	1	0	0.000000	-2.436962	1.833004		9	1	0	0.000000	-2.445801	1.843907
10	1	0	0.000000	2.436962	1.833004		10	1	0	0.000000	2.445801	1.843907
11	6	0	0.000000	-1.672813	-0.541176		11	6	0	0.000000	-1.653329	-0.514167
12	1	0	0.000000	-2.683152	-0.144681		12	1	0	0.000000	-2.669829	-0.135252
13	6	0	0.000000	1.672813	-0.541176		13	6	0	0.000000	1.653329	-0.514167
14	1	0	0.000000	2.683152	-0.144681		14	1	0	0.000000	2.669829	-0.135252
15	6	0	0.000000	-1.669698	-1.879548		15	6	0	0.000000	-1.655915	-1.917215
16	1	0	0.000000	-2.673495	-2.294897		16	1	0	0.000000	-2.669745	-2.306987
17	6	0	0.000000	1.669698	-1.879548		17	6	0	0.000000	1.655915	-1.917215
18	1	0	0.000000	2.673495	-2.294897		18	1	0	0.000000	2.669745	-2.306987
19	6	0	0.000000	-0.667793	-2.938050		19	6	0	0.000000	-0.711264	-2.914240
20	1	0	0.000000	-1.118578	-3.925853		20	1	0	0.000000	-1.134567	-3.913713
21	6	0	0.000000	0.667793	-2.938050		21	6	0	0.000000	0.711264	-2.914240
22	1	0	0.000000	1.118578	-3.925853		22	1	0	0.000000	1.134567	-3.913713
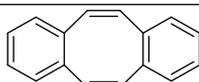
	S_0			T_1	
	E = -616.664116 a.u.			E = -616.6056108 a.u.	

Center Number	Atomic Number	Atomic Type	X	Y	Z		Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	0.690910	4.258603		1	6	0	0.000000	0.709255	-4.244635
2	6	0	0.000000	-0.690910	4.258603		2	6	0	0.000000	-0.709255	-4.244635
3	6	0	0.000000	-1.357497	3.044993		3	6	0	0.000000	-1.372679	-3.060581
4	6	0	0.000000	-0.704704	1.805526		4	6	0	0.000000	-0.722717	-1.780320
5	6	0	0.000000	0.704704	1.805526		5	6	0	0.000000	0.722717	-1.780320
6	6	0	0.000000	1.357497	3.044993		6	6	0	0.000000	1.372679	-3.060581
7	1	0	0.000000	1.250230	5.186000		7	1	0	0.000000	1.257113	-5.178755
8	1	0	0.000000	-1.250230	5.186000		8	1	0	0.000000	-1.257113	-5.178755
9	1	0	0.000000	-2.440999	3.050181		9	1	0	0.000000	-2.456110	-3.064551
10	1	0	0.000000	2.440999	3.050181		10	1	0	0.000000	2.456110	-3.064551
11	6	0	0.000000	-1.640555	0.669389		11	6	0	0.000000	-1.621747	-0.698523
12	1	0	0.000000	-2.656770	1.051668		12	1	0	0.000000	-2.645378	-1.059464
13	6	0	0.000000	1.640555	0.669389		13	6	0	0.000000	1.621747	-0.698523
14	1	0	0.000000	2.656770	1.051668		14	1	0	0.000000	2.645378	-1.059464
15	6	0	0.000000	-1.640555	-0.669389		15	6	0	0.000000	-1.621747	0.698523
16	1	0	0.000000	-2.656770	-1.051668		16	1	0	0.000000	-2.645378	1.059464
17	6	0	0.000000	1.640555	-0.669389		17	6	0	0.000000	1.621747	0.698523
18	1	0	0.000000	2.656770	-1.051668		18	1	0	0.000000	2.645378	1.059464
19	6	0	0.000000	-0.704704	-1.805526		19	6	0	0.000000	-0.722717	1.780320
20	6	0	0.000000	0.704704	-1.805526		20	6	0	0.000000	0.722717	1.780320
21	6	0	0.000000	1.357497	-3.044993		21	6	0	0.000000	1.372679	3.060581
22	1	0	0.000000	2.440999	-3.050181		22	1	0	0.000000	2.456110	3.064551
23	6	0	0.000000	-1.357497	-3.044993		23	6	0	0.000000	-1.372679	3.060581
24	1	0	0.000000	-2.440999	-3.050181		24	1	0	0.000000	-2.456110	3.064551
25	6	0	0.000000	0.690910	-4.258603		25	6	0	0.000000	0.709255	4.244635
26	1	0	0.000000	1.250230	-5.186000		26	1	0	0.000000	1.257113	5.178755
27	6	0	0.000000	-0.690910	-4.258603		27	6	0	0.000000	-0.709255	4.244635
28	1	0	0.000000	-1.250230	-5.186000		28	1	0	0.000000	-1.257113	5.178755

	S₀					

	S$_0$				

E = -616.6547492 a.u. (S$_0$)   **E = -616.6149119 a.u.** (T$_1$)
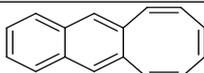
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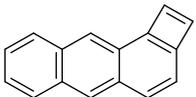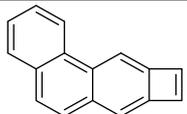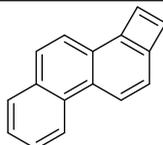<tr><td>Center Number</td><td>Atomic Number</td><td>Atomic Type</td><td colspan="3">Coordinates (Angstroms)
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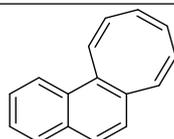
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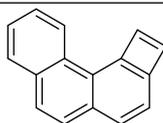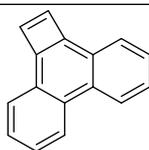<tr><td>Center Number</td><td>Atomic Number</td><td>Atomic Type</td><td colspan="3">Coordinates (Angstroms)
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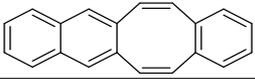
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5	6	0	0.000000	-1.397109	4.298521
6	6	0	0.000000	-0.705694	5.479699
7	1	0	0.000000	2.447480	1.826696
8	1	0	0.000000	1.239634	6.422328
9	1	0	0.000000	2.481420	4.294391
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28	1	0	0.000000	-2.441429	-4.261807
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Center Number	Atomic Number	Atomic Type	X	Y	Z
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5	6	0	-4.242320	1.623951	0.000000
6	6	0	-4.709124	2.902103	0.000000
7	1	0	0.110896	3.050146	0.000000
8	1	0	-4.197459	5.010278	0.000000
9	1	0	-1.768581	4.622954	0.000000
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13	1	0	-5.775864	3.091289	0.000000
14	6	0	-0.910218	-0.207936	0.000000
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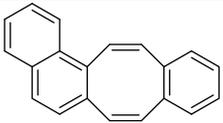
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3	6	0	0.689682	3.312730	0.000000

Center Number	Atomic Number	Atomic Type	X	Y	Z
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5	6	0	-1.671904	2.837301	0.000000
6	6	0	-1.944873	4.177217	0.000000
7	1	0	2.821266	3.641332	0.000000
8	1	0	-1.139717	6.188422	0.000000
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11	6	0	0.000000	0.914299	0.000000
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14	6	0	1.342577	0.551564	0.000000
15	6	0	2.331958	1.573579	0.000000
16	1	0	3.372236	1.273305	0.000000
17	6	0	-1.152725	-0.000370	0.000000
18	1	0	-2.070268	0.560145	0.000000
19	6	0	-1.464396	-1.305950	0.000000
20	1	0	-2.543044	-1.432208	0.000000
21	6	0	1.974496	-0.783873	0.000000
22	1	0	3.051118	-0.650110	0.000000
23	6	0	1.682380	-2.090230	0.000000
24	1	0	2.589574	-2.687117	0.000000
25	6	0	0.517261	-2.984746	0.000000
26	6	0	-0.845990	-2.641662	0.000000
27	6	0	0.855652	-4.341978	0.000000
28	6	0	-1.781592	-3.682315	0.000000
29	1	0	-2.833939	-3.423792	0.000000
30	6	0	-1.427240	-5.022307	0.000000
31	1	0	-2.193916	-5.787237	0.000000
32	6	0	-0.087289	-5.357840	0.000000
33	1	0	0.228651	-6.393745	0.000000
34	1	0	1.906440	-4.606833	0.000000

4	6	0	-0.259858	2.360757	0.000000
5	6	0	-1.549162	2.925604	0.000000
6	6	0	-1.761696	4.290517	0.000000
7	1	0	2.978193	3.499434	0.000000
8	1	0	-0.853077	6.245644	0.000000
9	1	0	1.446675	5.322593	0.000000
10	6	0	2.163132	2.785299	0.000000
11	6	0	0.000000	0.890428	0.000000
12	1	0	-2.432978	2.306965	0.000000
13	1	0	-2.777670	4.666656	0.000000
14	6	0	1.391889	0.452159	0.000000
15	6	0	2.412125	1.463190	0.000000
16	1	0	3.441165	1.125935	0.000000
17	6	0	-1.124012	0.077409	0.000000
18	1	0	-2.031242	0.657506	0.000000
19	6	0	-1.509329	-1.276024	0.000000
20	1	0	-2.593231	-1.332659	0.000000
21	6	0	1.938799	-0.846592	0.000000
22	1	0	3.021849	-0.782451	0.000000
23	6	0	1.573591	-2.181790	0.000000
24	1	0	2.460558	-2.807509	0.000000
25	6	0	0.403884	-2.990771	0.000000
26	6	0	-0.965233	-2.581463	0.000000
27	6	0	0.671668	-4.387541	0.000000
28	6	0	-1.954439	-3.612651	0.000000
29	1	0	-2.994090	-3.307329	0.000000
30	6	0	-1.655010	-4.943261	0.000000
31	1	0	-2.447502	-5.681361	0.000000
32	6	0	-0.305756	-5.342460	0.000000
33	1	0	-0.042427	-6.392952	0.000000
34	1	0	1.709790	-4.698117	0.000000

S_0					
E = -770.2390129 a.u.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	-0.710234	5.491759
2	6	0	0.000000	-1.398815	4.318265
3	6	0	0.000000	-0.714995	3.068418
4	6	0	0.000000	0.714995	3.068418
5	6	0	0.000000	1.398815	4.318265
6	6	0	0.000000	0.710234	5.491759
7	6	0	0.000000	-1.397201	1.846797
8	6	0	0.000000	1.397201	1.846797
9	6	0	0.000000	0.710980	0.643027
10	6	0	0.000000	-0.710980	0.643027
11	6	0	0.000000	-1.364881	-0.624177
12	1	0	0.000000	-2.448921	-0.609808
13	6	0	0.000000	-0.729524	-1.836459
14	6	0	0.000000	0.729524	-1.836459
15	6	0	0.000000	1.364881	-0.624177
16	1	0	0.000000	-2.482354	1.845494
17	1	0	0.000000	-1.242425	6.435404
18	1	0	0.000000	-2.483136	4.315466
19	1	0	0.000000	2.483136	4.315466
20	1	0	0.000000	1.242425	6.435404
21	1	0	0.000000	2.482354	1.845494
22	1	0	0.000000	2.448921	-0.609808
23	6	0	0.000000	1.675778	-2.964502
24	1	0	0.000000	2.689418	-2.576483
25	6	0	0.000000	-1.675778	-2.964502
26	1	0	0.000000	-2.689418	-2.576483
27	6	0	0.000000	-1.666048	-4.307792
28	1	0	0.000000	-2.669958	-4.723076

T_1					
E = -770.1965447 a.u.					
Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	0.712310	5.491619
2	6	0	0.000000	1.400781	4.321008
3	6	0	0.000000	0.717711	3.066585
4	6	0	0.000000	-0.717711	3.066585
5	6	0	0.000000	-1.400781	4.321008
6	6	0	0.000000	-0.712310	5.491619
7	6	0	0.000000	1.398878	1.853035
8	6	0	0.000000	-1.398878	1.853035
9	6	0	0.000000	-0.713897	0.637714
10	6	0	0.000000	0.713897	0.637714
11	6	0	0.000000	1.368541	-0.610232
12	1	0	0.000000	2.452348	-0.594892
13	6	0	0.000000	0.736325	-1.850665
14	6	0	0.000000	-0.736325	-1.850665
15	6	0	0.000000	-1.368541	-0.610232
16	1	0	0.000000	2.483899	1.852625
17	1	0	0.000000	1.243316	6.435890
18	1	0	0.000000	2.485026	4.318999
19	1	0	0.000000	-2.485026	4.318999
20	1	0	0.000000	-1.243316	6.435890
21	1	0	0.000000	-2.483899	1.852625
22	1	0	0.000000	-2.452348	-0.594892
23	6	0	0.000000	-1.659632	-2.939535
24	1	0	0.000000	-2.678729	-2.568238
25	6	0	0.000000	1.659632	-2.939535
26	1	0	0.000000	2.678729	-2.568238
27	6	0	0.000000	1.656202	-4.353552
28	1	0	0.000000	2.671184	-4.740777

29	6	0	0.000000	1.666048	-4.307792
30	1	0	0.000000	2.669958	-4.723076
31	6	0	0.000000	0.670074	-5.358597
32	1	0	0.000000	1.118755	-6.347423
33	6	0	0.000000	-0.670074	-5.358597
34	1	0	0.000000	-1.118755	-6.347423

29	6	0	0.000000	-1.656202	-4.353552
30	1	0	0.000000	-2.671184	-4.740777
31	6	0	0.000000	-0.720118	-5.342612
32	1	0	0.000000	-1.139132	-6.343800
33	6	0	0.000000	0.720118	-5.342612
34	1	0	0.000000	1.139132	-6.343800
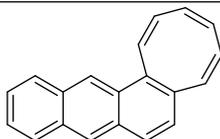
S_0	T_1
E = -770.2198264 a.u.	E = -770.1980943 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	3.384821	4.046827	0.000000
2	6	0	2.027417	4.020722	0.000000
3	6	0	1.323745	2.778149	0.000000
4	6	0	2.065928	1.560108	0.000000
5	6	0	3.493574	1.632847	0.000000
6	6	0	4.130194	2.832069	0.000000
7	6	0	-0.060064	2.690818	0.000000
8	6	0	1.399118	0.337101	0.000000
9	6	0	0.000000	0.221375	0.000000
10	6	0	-0.722047	1.464946	0.000000
11	6	0	-2.135733	1.428265	0.000000
12	1	0	-2.690171	2.359431	0.000000
13	6	0	-2.779348	0.241200	0.000000
14	6	0	-2.110414	-1.024735	0.000000
15	6	0	-0.726073	-1.051909	0.000000
16	1	0	-0.653216	3.599289	0.000000
17	1	0	3.912366	4.993076	0.000000
18	1	0	1.455455	4.941810	0.000000
19	1	0	4.060222	0.708306	0.000000
20	1	0	5.212727	2.873988	0.000000
21	1	0	2.041120	-0.528836	0.000000
22	1	0	-3.861731	0.239315	0.000000
23	6	0	0.154131	-2.247005	0.000000
24	1	0	1.187877	-1.953845	0.000000
25	6	0	0.085349	-3.585813	0.000000
26	1	0	1.072785	-4.039382	0.000000
27	6	0	-3.122394	-2.119840	0.000000
28	1	0	-4.111275	-1.674939	0.000000
29	6	0	-3.207535	-3.454421	0.000000
30	1	0	-4.236659	-3.802198	0.000000
31	6	0	-0.943060	-4.622504	0.000000
32	1	0	-0.518226	-5.621569	0.000000
33	6	0	-2.273794	-4.574339	0.000000
34	1	0	-2.774166	-5.537618	0.000000

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	2.961726	4.377125	0.000000
2	6	0	1.609583	4.204442	0.000000
3	6	0	1.048217	2.899534	0.000000
4	6	0	1.911173	1.772890	0.000000
5	6	0	3.316599	1.990190	0.000000
6	6	0	3.827085	3.254120	0.000000
7	6	0	-0.329518	2.658194	0.000000
8	6	0	1.365468	0.478367	0.000000
9	6	0	0.000000	0.221490	0.000000
10	6	0	-0.850307	1.378892	0.000000
11	6	0	-2.268187	1.192967	0.000000
12	1	0	-2.909232	2.066660	0.000000
13	6	0	-2.796102	-0.042793	0.000000
14	6	0	-2.023567	-1.259162	0.000000
15	6	0	-0.589729	-1.149178	0.000000
16	1	0	-1.014750	3.499436	0.000000
17	1	0	3.383287	5.375089	0.000000
18	1	0	0.943526	5.059997	0.000000
19	1	0	3.977966	1.130762	0.000000
20	1	0	4.899475	3.407526	0.000000
21	1	0	2.093885	-0.317816	0.000000
22	1	0	-3.873960	-0.144884	0.000000
23	6	0	0.351306	-2.197539	0.000000
24	1	0	1.360564	-1.824959	0.000000
25	6	0	0.421554	-3.600319	0.000000
26	1	0	1.456894	-3.928774	0.000000
27	6	0	-2.882894	-2.396330	0.000000
28	1	0	-3.917565	-2.071636	0.000000
29	6	0	-2.837597	-3.787352	0.000000
30	1	0	-3.835742	-4.215034	0.000000
31	6	0	-0.453026	-4.673575	0.000000
32	1	0	0.046169	-5.637356	0.000000
33	6	0	-1.845683	-4.759248	0.000000
34	1	0	-2.227124	-5.775297	0.000000
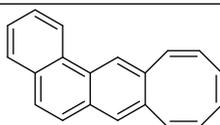
S_0	T_1
E = -770.245971 a.u.	E = -770.2089697 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-2.621176	-2.415160	0.000000
2	6	0	-1.280771	-2.585402	0.000000
3	6	0	-0.405218	-1.456210	0.000000

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-2.652805	-2.374743	0.000000
2	6	0	-1.319726	-2.567919	0.000000
3	6	0	-0.416222	-1.453392	0.000000

Center Number	Atomic Number	Atomic Type	X	Y	Z		Center Number	Atomic Number	Atomic Type	X	Y	Z
4	6	0	-0.928831	-0.158107	0.000000		4	6	0	-0.925675	-0.130616	0.000000
5	6	0	-2.364787	0.034286	0.000000		5	6	0	-2.368728	0.077891	0.000000
6	6	0	-3.201888	-1.106404	0.000000		6	6	0	-3.218255	-1.050821	0.000000
7	1	0	1.372677	-2.628767	0.000000		7	1	0	1.322240	-2.658609	0.000000
8	1	0	-3.285681	-3.271753	0.000000		8	1	0	-3.332027	-3.219735	0.000000
9	1	0	-0.848869	-3.579660	0.000000		9	1	0	-0.905288	-3.569654	0.000000
10	6	0	0.994364	-1.612810	0.000000		10	6	0	0.959484	-1.637033	0.000000
11	6	0	0.000000	0.901140	0.000000		11	6	0	0.000000	0.901673	0.000000
12	6	0	1.375462	0.755790	0.000000		12	6	0	1.401195	0.746877	0.000000
13	6	0	1.904634	-0.575490	0.000000		13	6	0	1.913769	-0.606876	0.000000
14	1	0	-0.383453	1.911691	0.000000		14	1	0	-0.365818	1.918830	0.000000
15	6	0	2.072497	2.059705	0.000000		15	6	0	2.087841	1.999290	0.000000
16	1	0	1.337193	2.857909	0.000000		16	1	0	1.379271	2.820538	0.000000
17	6	0	3.302900	-1.055853	0.000000		17	6	0	3.256883	-1.100064	0.000000
18	1	0	3.306327	-2.141177	0.000000		18	1	0	3.259983	-2.184848	0.000000
19	6	0	3.322077	2.544735	0.000000		19	6	0	3.405749	2.494001	0.000000
20	1	0	3.341043	3.630849	0.000000		20	1	0	3.412760	3.580228	0.000000
21	6	0	4.547716	-0.559376	0.000000		21	6	0	4.572375	-0.606343	0.000000
22	1	0	5.302504	-1.340571	0.000000		22	1	0	5.293782	-1.418431	0.000000
23	6	0	4.670486	2.001922	0.000000		23	6	0	4.667052	1.963270	0.000000
24	6	0	5.161924	0.758085	0.000000		24	6	0	5.170965	0.625891	0.000000
25	1	0	6.246255	0.702691	0.000000		25	1	0	6.255529	0.583903	0.000000
26	1	0	5.424306	2.783327	0.000000		26	1	0	5.454483	2.710261	0.000000
27	6	0	-2.974042	1.305663	0.000000		27	6	0	-2.960412	1.352910	0.000000
28	1	0	-2.363706	2.198494	0.000000		28	1	0	-2.339215	2.238438	0.000000
29	6	0	-4.601413	-0.942317	0.000000		29	6	0	-4.611913	-0.871827	0.000000
30	1	0	-5.228480	-1.826907	0.000000		30	1	0	-5.249480	-1.748959	0.000000
31	6	0	-5.166007	0.307026	0.000000		31	6	0	-5.164969	0.386446	0.000000
32	1	0	-6.243231	0.420566	0.000000		32	1	0	-6.241004	0.510871	0.000000
33	6	0	-4.340304	1.441008	0.000000		33	6	0	-4.328056	1.507210	0.000000
34	1	0	-4.782620	2.429913	0.000000		34	1	0	-4.756527	2.502223	0.000000
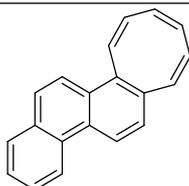
	S$_0$	T$_1$
	E = -770.2292773 a.u.	E = -770.2012214 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z		Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-2.695148	1.553421	0.000000		1	6	0	-2.657679	1.626346	0.000000
2	6	0	-2.493490	0.161664	0.000000		2	6	0	-2.478208	0.227911	0.000000
3	6	0	-1.133617	-0.364364	0.000000		3	6	0	-1.135779	-0.317622	0.000000
4	6	0	0.000000	0.497919	0.000000		4	6	0	0.000000	0.514633	0.000000
5	6	0	-0.292291	1.915242	0.000000		5	6	0	-0.253303	1.929180	0.000000
6	6	0	-1.548717	2.403819	0.000000		6	6	0	-1.501392	2.451558	0.000000
7	1	0	-1.729113	-2.438545	0.000000		7	1	0	-1.782052	-2.394025	0.000000
8	6	0	-0.906436	-1.739070	0.000000		8	6	0	-0.938400	-1.720589	0.000000
9	6	0	1.342856	-0.030160	0.000000		9	6	0	1.365821	-0.044872	0.000000
10	1	0	0.496449	2.647322	0.000000		10	1	0	0.554262	2.641543	0.000000
11	1	0	-1.704154	3.476998	0.000000		11	1	0	-1.631359	3.528011	0.000000
12	6	0	1.517531	-1.421551	0.000000		12	6	0	1.504713	-1.472753	0.000000
13	6	0	0.368641	-2.231291	0.000000		13	6	0	0.307181	-2.246378	0.000000
14	1	0	0.498685	-3.305987	0.000000		14	1	0	0.407827	-3.324371	0.000000
15	6	0	2.416004	0.994675	0.000000		15	6	0	2.411640	0.911972	0.000000
16	1	0	1.996904	1.982872	0.000000		16	1	0	2.034144	1.917509	0.000000
17	6	0	3.753909	1.100555	0.000000		17	6	0	3.818485	0.994160	0.000000
18	1	0	4.070669	2.140082	0.000000		18	1	0	4.133949	2.033721	0.000000
19	6	0	2.741068	-2.271550	0.000000		19	6	0	2.656405	-2.323689	0.000000
20	1	0	2.433041	-3.311407	0.000000		20	1	0	2.340302	-3.360881	0.000000
21	6	0	4.075438	-2.176404	0.000000		21	6	0	4.051415	-2.264315	0.000000
22	1	0	4.558290	-3.149445	0.000000		22	1	0	4.488086	-3.258704	0.000000
23	6	0	5.055928	-1.100529	0.000000		23	6	0	5.003307	-1.267192	0.000000
24	1	0	6.079093	-1.463018	0.000000		24	1	0	6.026127	-1.629807	0.000000

25	6	0	4.919978	0.225109	0.000000
26	1	0	5.851243	0.783066	0.000000
27	6	0	-3.635292	-0.665089	0.000000
28	1	0	-3.532698	-1.740754	0.000000
29	6	0	-3.998533	2.083309	0.000000
30	1	0	-4.123312	3.160393	0.000000
31	6	0	-5.091883	1.255100	0.000000
32	1	0	-6.093435	1.667512	0.000000
33	6	0	-4.902734	-0.133249	0.000000
34	1	0	-5.760931	-0.794433	0.000000

25	6	0	4.895282	0.138535	0.000000
26	1	0	5.854076	0.647290	0.000000
27	6	0	-3.638883	-0.579599	0.000000
28	1	0	-3.556411	-1.656787	0.000000
29	6	0	-3.955166	2.177989	0.000000
30	1	0	-4.061644	3.257055	0.000000
31	6	0	-5.059760	1.369006	0.000000
32	1	0	-6.054737	1.797161	0.000000
33	6	0	-4.893766	-0.025446	0.000000
34	1	0	-5.764040	-0.670727	0.000000
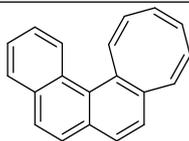
S₀	T₁

S_0 — E = -770.2508027 a.u.

T_1 — E = -770.1976355 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-3.037498	1.716657	0.162123
2	6	0	-1.952262	2.505005	0.256254
3	6	0	-0.630683	1.966474	0.134071
4	6	0	-0.421570	0.584163	-0.088763
5	6	0	-1.601641	-0.285782	-0.040900
6	6	0	-2.892805	0.299807	0.030746
7	1	0	0.273239	3.901907	0.370850
8	1	0	-4.036858	2.132069	0.223014
9	1	0	-2.053449	3.574633	0.400396
10	6	0	0.460504	2.849847	0.188660
11	6	0	0.915969	0.139195	-0.359855
12	6	0	1.975016	1.039033	-0.291778
13	6	0	1.730466	2.395160	-0.003938
14	1	0	2.568565	3.081444	0.032829
15	6	0	1.167983	-1.218280	-0.909087
16	1	0	0.587846	-1.455722	-1.797564
17	6	0	1.969109	-2.164888	-0.428980
18	1	0	1.988660	-3.120571	-0.949169
19	6	0	3.395048	0.719886	-0.578928
20	1	0	3.875787	1.416330	-1.261415
21	6	0	4.176222	-0.184181	0.009780
22	1	0	5.237312	-0.158225	-0.227700
23	6	0	3.774472	-1.206549	0.978657
24	1	0	4.387073	-1.296210	1.871777
25	6	0	2.795102	-2.088324	0.782618
26	1	0	2.641867	-2.870019	1.522780
27	6	0	-1.548518	-1.696282	0.003489
28	1	0	-0.595654	-2.192992	0.047259
29	6	0	-4.043231	-0.511334	0.036097
30	1	0	-5.012932	-0.027464	0.072453
31	6	0	-3.951279	-1.879135	0.022088
32	1	0	-4.844573	-2.491894	0.032185
33	6	0	-2.684704	-2.471036	0.029872
34	1	0	-2.591088	-3.549890	0.068953

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	3.230126	1.465178	0.283028
2	6	0	2.230347	2.375250	0.256603
3	6	0	0.870810	1.969835	0.131234
4	6	0	0.527228	0.611327	0.084055
5	6	0	1.605525	-0.348704	-0.075927
6	6	0	2.949263	0.083494	0.075524
7	1	0	0.110692	3.997305	0.089209
8	1	0	4.261442	1.774810	0.407323
9	1	0	2.443040	3.434426	0.346721
10	6	0	-0.156813	2.947818	0.053173
11	6	0	-0.872977	0.218936	0.197728
12	6	0	-1.867239	1.204351	-0.128375
13	6	0	-1.441625	2.569942	-0.142820
14	1	0	-2.200167	3.327808	-0.297674
15	6	0	-1.097371	-1.024142	0.847996
16	1	0	-0.203004	-1.363065	1.355354
17	6	0	-2.145804	-1.930355	1.044296
18	1	0	-1.855378	-2.735877	1.712660
19	6	0	-3.233672	1.048685	-0.478491
20	1	0	-3.674649	2.005367	-0.740724
21	6	0	-4.137754	0.003549	-0.705623
22	1	0	-5.022352	0.344212	-1.236408
23	6	0	-4.207483	-1.325493	-0.343060
24	1	0	-5.106118	-1.828981	-0.685615
25	6	0	-3.403503	-2.115205	0.503931
26	1	0	-3.866380	-3.055839	0.786282
27	6	0	1.403238	-1.689417	-0.484684
28	1	0	0.404651	-2.028132	-0.718977
29	6	0	4.005753	-0.843125	-0.049791
30	1	0	5.020687	-0.491062	0.097548
31	6	0	3.766677	-2.149563	-0.382374
32	1	0	4.587364	-2.849016	-0.485881
33	6	0	2.449384	-2.564496	-0.631664
34	1	0	2.255515	-3.579144	-0.958361
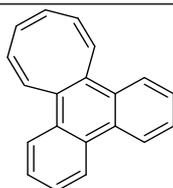
S₀	T₁

S_0 — E = -770.2115954 a.u.

T_1 — E = -770.1895661 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.514249	-1.794964	1	6	0	0.000000	3.521390	-1.805638
2	6	0	0.000000	-2.841058	-0.601861	2	6	0	0.000000	2.849298	-0.607449
3	6	0	0.000000	-1.420562	-0.512219	3	6	0	0.000000	1.435679	-0.510512
4	6	0	0.000000	-0.722463	-1.741882	4	6	0	0.000000	0.730316	-1.731176
5	6	0	0.000000	-1.440705	-2.957069	5	6	0	0.000000	1.438053	-2.946433
6	6	0	0.000000	-2.807440	-2.997819	6	6	0	0.000000	2.809217	-2.999749
7	6	0	0.000000	-0.688803	0.764583	7	6	0	0.000000	0.716079	0.792576
8	6	0	0.000000	0.722463	-1.741882	8	6	0	0.000000	-0.730316	-1.731176
9	6	0	0.000000	1.420562	-0.512219	9	6	0	0.000000	-1.435679	-0.510512
10	6	0	0.000000	0.688803	0.764583	10	6	0	0.000000	-0.716079	0.792576
11	6	0	0.000000	2.841058	-0.601861	11	6	0	0.000000	-2.849298	-0.607449
12	1	0	0.000000	3.465544	0.273816	12	1	0	0.000000	-3.476799	0.267182
13	6	0	0.000000	3.514249	-1.794964	13	6	0	0.000000	-3.521390	-1.805638
14	6	0	0.000000	2.807440	-2.997819	14	6	0	0.000000	-2.809217	-2.999749
15	6	0	0.000000	1.440705	-2.957069	15	6	0	0.000000	-1.438053	-2.946433
16	1	0	0.000000	-4.597481	-1.794565	16	1	0	0.000000	4.604645	-1.808346
17	1	0	0.000000	-3.465544	0.273816	17	1	0	0.000000	3.476799	0.267182
18	1	0	0.000000	-0.908824	-3.895156	18	1	0	0.000000	0.901903	-3.882020
19	1	0	0.000000	-3.328251	-3.947394	19	1	0	0.000000	3.320542	-3.954478
20	1	0	0.000000	4.597481	-1.794565	20	1	0	0.000000	-4.604645	-1.808346
21	1	0	0.000000	3.328251	-3.947394	21	1	0	0.000000	-3.320542	-3.954478
22	1	0	0.000000	0.908824	-3.895156	22	1	0	0.000000	-0.901903	-3.882020
23	6	0	0.000000	1.597030	1.947235	23	6	0	0.000000	-1.580260	1.917740
24	1	0	0.000000	2.615019	1.615637	24	1	0	0.000000	-2.605616	1.605724
25	6	0	0.000000	-1.597030	1.947235	25	6	0	0.000000	1.580260	1.917740
26	1	0	0.000000	-2.615019	1.615637	26	1	0	0.000000	2.605616	1.605724
27	6	0	0.000000	-1.616097	3.288317	27	6	0	0.000000	1.604400	3.319167
28	1	0	0.000000	-2.633295	3.671139	28	1	0	0.000000	2.629223	3.679656
29	6	0	0.000000	1.616097	3.288317	29	6	0	0.000000	-1.604400	3.319167
30	1	0	0.000000	2.633295	3.671139	30	1	0	0.000000	-2.629223	3.679656
31	6	0	0.000000	0.664331	4.390882	31	6	0	0.000000	-0.697034	4.362275
32	1	0	0.000000	1.142176	5.365307	32	1	0	0.000000	-1.152019	5.347479
33	6	0	0.000000	-0.664331	4.390882	33	6	0	0.000000	0.697034	4.362275
34	1	0	0.000000	-1.142176	5.365307	34	1	0	0.000000	1.152019	5.347479
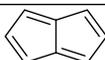
	S_0						T_1				
	E = -308.2619637 a.u.						E = -308.2448996 a.u.				
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.159601	1.411035	0.000000	1	6	0	0.000000	1.165975	1.332621
2	6	0	-0.729054	0.002262	0.000000	2	6	0	0.000000	0.739459	0.000000
3	6	0	0.729054	-0.002262	0.000000	3	6	0	0.000000	-0.739459	0.000000
4	6	0	1.159601	1.269922	0.000000	4	6	0	0.000000	-1.165975	1.332621
5	1	0	0.005202	3.239587	0.000000	5	1	0	0.000000	0.000000	3.216082
6	1	0	-2.177796	1.770723	0.000000	6	1	0	0.000000	2.180886	1.700715
7	1	0	2.180930	1.627595	0.000000	7	1	0	0.000000	-2.180886	1.700715
8	6	0	-0.042239	2.159740	0.000000	8	6	0	0.000000	0.000000	2.133853
9	6	0	1.159601	-1.411035	0.000000	9	6	0	0.000000	-1.165975	-1.332621
10	1	0	2.177796	-1.770723	0.000000	10	1	0	0.000000	-2.180886	-1.700715
11	6	0	-1.159601	-1.269922	0.000000	11	6	0	0.000000	1.165975	-1.332621
12	1	0	-2.180930	-1.627595	0.000000	12	1	0	0.000000	2.180886	-1.700715
13	6	0	0.042239	-2.159740	0.000000	13	6	0	0.000000	0.000000	-2.133853
14	1	0	-0.005202	-3.239587	0.000000	14	1	0	0.000000	0.000000	-3.216082

	S₀
	E = -461.8764742 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.710687	0.000000
2	6	0	1.101116	-0.262467	0.000000
3	6	0	0.496668	-1.598774	0.000000
4	6	0	-0.842970	-1.491827	0.000000
5	1	0	-1.570854	-2.293067	0.000000
6	6	0	-1.196368	-0.050674	0.000000
7	6	0	1.591469	-2.569575	0.000000
8	1	0	1.496809	-3.644820	0.000000
9	6	0	2.438096	-0.402819	0.000000
10	1	0	3.191054	0.373291	0.000000
11	6	0	2.737564	-1.857977	0.000000
12	1	0	3.738283	-2.267583	0.000000
13	6	0	-2.424658	0.569721	0.000000
14	1	0	-3.341798	-0.008181	0.000000
15	6	0	-0.052304	2.084542	0.000000
16	1	0	0.854352	2.677895	0.000000
17	6	0	-2.471954	1.971036	0.000000
18	1	0	-3.431046	2.474419	0.000000
19	6	0	-1.306254	2.713534	0.000000
20	1	0	-1.359223	3.795604	0.000000

	T₁
	E = -461.8451169 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.665390	0.000000
2	6	0	1.067450	-0.278888	0.000000
3	6	0	0.490285	-1.617786	0.000000
4	6	0	-0.905512	-1.507576	0.000000
5	1	0	-1.632271	-2.306502	0.000000
6	6	0	-1.218179	-0.094362	0.000000
7	6	0	1.545468	-2.522229	0.000000
8	1	0	1.495525	-3.601167	0.000000
9	6	0	2.491476	-0.397494	0.000000
10	1	0	3.211465	0.406742	0.000000
11	6	0	2.777238	-1.739967	0.000000
12	1	0	3.769811	-2.169260	0.000000
13	6	0	-2.438851	0.569561	0.000000
14	1	0	-3.369823	0.014758	0.000000
15	6	0	-0.035107	2.058104	0.000000
16	1	0	0.884116	2.632027	0.000000
17	6	0	-2.451262	1.959590	0.000000
18	1	0	-3.400338	2.482640	0.000000
19	6	0	-1.264540	2.698954	0.000000
20	1	0	-1.309274	3.780979	0.000000

	S₀
	E = -615.4877752 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.189813	3.348104	0.000000
2	6	0	0.773962	2.031954	0.000000
3	6	0	-0.607224	1.716768	0.000000
4	6	0	-1.554168	2.718381	0.000000
5	6	0	-1.126598	4.049435	0.000000
6	6	0	0.224473	4.358917	0.000000
7	1	0	2.244477	3.598673	0.000000
8	1	0	-2.612424	2.484773	0.000000
9	1	0	-1.859526	4.847149	0.000000
10	1	0	0.536310	5.396480	0.000000
11	6	0	-0.689872	0.254095	0.000000
12	6	0	1.554168	0.775270	0.000000
13	1	0	2.635297	0.733533	0.000000
14	6	0	0.689872	-0.254095	0.000000
15	6	0	0.607224	-1.716768	0.000000
16	6	0	-1.554168	-0.775270	0.000000
17	1	0	-2.635297	-0.733533	0.000000
18	6	0	-0.773962	-2.031954	0.000000
19	6	0	1.554168	-2.718381	0.000000
20	1	0	2.612424	-2.484773	0.000000
21	6	0	-1.189813	-3.348104	0.000000
22	1	0	-2.244477	-3.598673	0.000000
23	6	0	-0.224473	-4.358917	0.000000
24	1	0	-0.536310	-5.396480	0.000000
25	6	0	1.126598	-4.049435	0.000000
26	1	0	1.859526	-4.847149	0.000000

	T₁
	E = -615.4313994 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.573763	-0.197415	0.000000
2	6	0	2.157373	-0.028685	0.000000
3	6	0	1.300627	-1.213143	0.000000
4	6	0	1.875026	-2.485439	0.000000
5	6	0	3.248067	-2.604110	0.000000
6	6	0	4.092913	-1.456772	0.000000
7	1	0	4.220396	0.672171	0.000000
8	1	0	1.248358	-3.369326	0.000000
9	1	0	3.702544	-3.587518	0.000000
10	1	0	5.166807	-1.599767	0.000000
11	6	0	-0.051797	-0.752811	0.000000
12	6	0	1.387192	1.122618	0.000000
13	1	0	1.754563	2.137916	0.000000
14	6	0	0.000000	0.694601	0.000000
15	6	0	-1.321840	1.190552	0.000000
16	6	0	-1.367153	-1.165596	0.000000
17	1	0	-1.751031	-2.174981	0.000000
18	6	0	-2.183633	0.038111	0.000000
19	6	0	-1.860479	2.482130	0.000000
20	1	0	-1.209878	3.349078	0.000000
21	6	0	-3.557496	0.217225	0.000000
22	1	0	-4.228091	-0.634351	0.000000
23	6	0	-4.071767	1.511895	0.000000
24	1	0	-5.146163	1.654651	0.000000
25	6	0	-3.235189	2.634563	0.000000
26	1	0	-3.671151	3.625781	0.000000
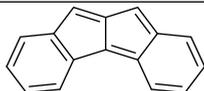
| | S$_0$ | | | | | T$_1$ | | | |
| | E = -615.4498031 a.u. | | | | | E = -615.452597 a.u. | | | |

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-3.616605	-0.126571	0.000000
2	6	0	-2.298198	0.265386	0.000000
3	6	0	-1.247856	-0.693208	0.000000
4	6	0	-1.547771	-2.036123	0.000000
5	6	0	-2.895045	-2.430978	0.000000
6	6	0	-3.913586	-1.497441	0.000000
7	1	0	-4.415332	0.606626	0.000000
8	1	0	-0.764993	-2.784912	0.000000
9	1	0	-3.137580	-3.487117	0.000000
10	1	0	-4.946064	-1.824262	0.000000
11	6	0	0.000000	0.073284	0.000000
12	6	0	-1.699165	1.615647	0.000000
13	1	0	-2.272052	2.534543	0.000000
14	6	0	-0.354581	1.484727	0.000000
15	6	0	0.870827	2.271367	0.000000
16	6	0	1.358368	-0.015563	0.000000
17	6	0	1.897853	1.375307	0.000000
18	6	0	3.322660	1.567753	0.000000
19	1	0	3.726391	2.573683	0.000000
20	6	0	2.282133	-1.114405	0.000000
21	1	0	1.912842	-2.132648	0.000000
22	6	0	4.135991	0.491323	0.000000
23	1	0	5.211445	0.621646	0.000000
24	6	0	3.608607	-0.859456	0.000000
25	1	0	4.314250	-1.682150	0.000000
26	1	0	0.949309	3.348304	0.000000

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	3.558748	0.715694
2	6	0	0.000000	2.179679	0.834567
3	6	0	0.000000	1.362900	-0.340439
4	6	0	0.000000	1.945137	-1.598884
5	6	0	0.000000	3.335399	-1.699668
6	6	0	0.000000	4.129125	-0.558246
7	1	0	0.000000	4.190213	1.596680
8	1	0	0.000000	1.334407	-2.493675
9	1	0	0.000000	3.802516	-2.676856
10	1	0	0.000000	5.207864	-0.659381
11	6	0	0.000000	0.000000	0.113855
12	6	0	0.000000	1.325087	2.010468
13	1	0	0.000000	1.673721	3.033067
14	6	0	0.000000	0.000000	1.559215
15	6	0	0.000000	-1.325087	2.010468
16	6	0	0.000000	-1.362900	-0.340439
17	6	0	0.000000	-2.179679	0.834567
18	6	0	0.000000	-3.558748	0.715694
19	1	0	0.000000	-4.190213	1.596680
20	6	0	0.000000	-1.945137	-1.598884
21	1	0	0.000000	-1.334407	-2.493675
22	6	0	0.000000	-4.129125	-0.558246
23	1	0	0.000000	-5.207864	-0.659381
24	6	0	0.000000	-3.335399	-1.699668
25	1	0	0.000000	-3.802516	-2.676856
26	1	0	0.000000	-1.673721	3.033067

| | S$_0$ | | | | | T$_1$ | | | |
| | E = -615.4703749 a.u. | | | | | E = -615.4354585 a.u. | | | |

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	0.786940	0.000000
2	6	0	1.256748	0.281029	0.000000
3	6	0	1.454012	-1.136923	0.000000
4	6	0	0.328847	-2.002558	0.000000
5	6	0	-0.987586	-1.442840	0.000000
6	6	0	-1.143692	-0.096107	0.000000
7	1	0	3.604026	-1.039792	0.000000
8	1	0	2.125830	0.929679	0.000000
9	6	0	2.745028	-1.701780	0.000000
10	6	0	0.539553	-3.395877	0.000000
11	1	0	-1.843053	-2.109975	0.000000
12	6	0	1.808498	-3.919076	0.000000
13	6	0	2.921995	-3.063063	0.000000
14	1	0	-0.322483	-4.054046	0.000000
15	1	0	1.953752	-4.992580	0.000000
16	1	0	3.921846	-3.480149	0.000000
17	6	0	-2.367418	0.728975	0.000000
18	1	0	-3.370110	0.320997	0.000000
19	6	0	-0.545994	2.145298	0.000000
20	6	0	-2.010499	2.026469	0.000000
21	6	0	-0.228875	3.454129	0.000000

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	0.785148	0.000000
2	6	0	1.240878	0.198379	0.000000
3	6	0	1.354680	-1.214809	0.000000
4	6	0	0.174342	-2.014655	0.000000
5	6	0	-1.106506	-1.394217	0.000000
6	6	0	-1.209787	-0.031678	0.000000
7	1	0	3.509943	-1.240265	0.000000
8	1	0	2.142646	0.800972	0.000000
9	6	0	2.616158	-1.854457	0.000000
10	6	0	0.313049	-3.420631	0.000000
11	1	0	-1.991529	-2.021261	0.000000
12	6	0	1.549764	-4.010454	0.000000
13	6	0	2.715961	-3.219626	0.000000
14	1	0	-0.582791	-4.031525	0.000000
15	1	0	1.634505	-5.090554	0.000000
16	1	0	3.689027	-3.695305	0.000000
17	6	0	-2.360288	0.842059	0.000000
18	1	0	-3.389996	0.516605	0.000000
19	6	0	-0.431027	2.140779	0.000000
20	6	0	-1.876737	2.160398	0.000000
21	6	0	0.047796	3.502767	0.000000

22	1	0	0.754631	3.902866	0.000000
23	6	0	-2.554925	3.378605	0.000000
24	1	0	-3.598962	3.652289	0.000000
25	6	0	-1.495443	4.218714	0.000000
26	1	0	-1.546970	5.299107	0.000000

22	1	0	1.077628	3.826584	0.000000
23	6	0	-2.270644	3.498073	0.000000
24	1	0	-3.277109	3.891133	0.000000
25	6	0	-1.052689	4.308593	0.000000
26	1	0	-1.042019	5.389604	0.000000

	S_0			
	E = -615.4622611 a.u.			

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.928987	-0.665347	0.000000
2	6	0	2.258385	-0.036815	0.000000
3	6	0	2.047420	1.411001	0.000000
4	6	0	0.728430	1.670007	0.000000
5	1	0	0.253513	2.641857	0.000000
6	6	0	0.000000	0.373211	0.000000
7	6	0	3.370158	2.043300	0.000000
8	1	0	3.575586	3.103131	0.000000
9	6	0	3.581340	-0.272289	0.000000
10	1	0	4.089914	-1.226920	0.000000
11	6	0	4.275326	1.045099	0.000000
12	1	0	5.350297	1.160678	0.000000
13	6	0	-1.383355	0.113689	0.000000
14	6	0	0.515735	-1.999719	0.000000
15	1	0	1.244211	-2.801770	0.000000
16	6	0	-1.799256	-1.252850	0.000000
17	6	0	-0.830596	-2.280716	0.000000
18	1	0	-1.170725	-3.310242	0.000000
19	6	0	-3.188613	-1.542257	0.000000
20	1	0	-3.501758	-2.580568	0.000000
21	6	0	-2.376219	1.129528	0.000000
22	1	0	-2.070760	2.168832	0.000000
23	6	0	-3.702790	0.810879	0.000000
24	1	0	-4.448302	1.597159	0.000000
25	6	0	-4.116374	-0.542218	0.000000
26	1	0	-5.173444	-0.779175	0.000000

	T_1			
	E = -615.4364122 a.u.			

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.953433	-0.629234	0.000000
2	6	0	2.237260	-0.026747	0.000000
3	6	0	2.050704	1.429631	0.000000
4	6	0	0.677133	1.697576	0.000000
5	1	0	0.203636	2.667514	0.000000
6	6	0	0.000000	0.429987	0.000000
7	6	0	3.309968	2.012207	0.000000
8	1	0	3.555836	3.063610	0.000000
9	6	0	3.622884	-0.297453	0.000000
10	1	0	4.103197	-1.264144	0.000000
11	6	0	4.268469	0.931364	0.000000
12	1	0	5.341599	1.068488	0.000000
13	6	0	-1.393325	0.133354	0.000000
14	6	0	0.537327	-1.979188	0.000000
15	1	0	1.274467	-2.773271	0.000000
16	6	0	-1.783770	-1.233665	0.000000
17	6	0	-0.793453	-2.267566	0.000000
18	1	0	-1.131163	-3.297456	0.000000
19	6	0	-3.158525	-1.544230	0.000000
20	1	0	-3.457813	-2.586409	0.000000
21	6	0	-2.391379	1.131453	0.000000
22	1	0	-2.097009	2.173725	0.000000
23	6	0	-3.721041	0.797420	0.000000
24	1	0	-4.476001	1.574198	0.000000
25	6	0	-4.108376	-0.553962	0.000000
26	1	0	-5.160606	-0.811939	0.000000

	S_0			
	E = -769.0801521 a.u.			

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	0.672227	0.000000
2	6	0	0.042996	2.028557	0.000000
3	6	0	-1.172962	2.776573	0.000000
4	6	0	-2.417914	2.091690	0.000000
5	6	0	-2.436178	0.664742	0.000000
6	6	0	-1.264639	-0.023620	0.000000
7	1	0	-0.220309	4.708192	0.000000
8	1	0	0.986816	2.562831	0.000000
9	6	0	-1.171687	4.187644	0.000000
10	6	0	-3.610058	2.847021	0.000000
11	1	0	-3.391445	0.150755	0.000000
12	6	0	-3.578217	4.217660	0.000000
13	6	0	-2.345927	4.895449	0.000000

	T_1			
	E = -769.0233179 a.u.			

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.000000	0.622600	0.000000
2	6	0	0.135768	1.987908	0.000000
3	6	0	-1.020558	2.814123	0.000000
4	6	0	-2.311391	2.211542	0.000000
5	6	0	-2.434306	0.788463	0.000000
6	6	0	-1.320633	0.002912	0.000000
7	1	0	0.062595	4.675694	0.000000
8	1	0	1.115835	2.452788	0.000000
9	6	0	-0.922628	4.222312	0.000000
10	6	0	-3.445524	3.047907	0.000000
11	1	0	-3.427555	0.352094	0.000000
12	6	0	-3.319451	4.415289	0.000000
13	6	0	-2.045476	5.009883	0.000000

14	1	0	-4.559439	2.322861	0.000000
15	1	0	-4.502880	4.782149	0.000000
16	1	0	-2.327298	5.978598	0.000000
17	6	0	-1.000709	-1.473252	0.000000
18	1	0	-1.775147	-2.228738	0.000000
19	6	0	1.028110	-0.367269	0.000000
20	6	0	0.330852	-1.662664	0.000000
21	6	0	2.358618	-0.565890	0.000000
22	1	0	3.140334	0.181630	0.000000
23	6	0	1.359637	-2.701001	0.000000
24	6	0	2.603376	-2.021592	0.000000
25	6	0	1.312252	-4.079974	0.000000
26	1	0	0.363971	-4.604764	0.000000
27	6	0	3.786521	-2.735730	0.000000
28	1	0	4.743534	-2.226661	0.000000
29	6	0	2.512016	-4.794404	0.000000
30	1	0	2.490784	-5.877420	0.000000
31	6	0	3.730588	-4.130693	0.000000
32	1	0	4.651034	-4.702276	0.000000

14	1	0	-4.429484	2.592133	0.000000
15	1	0	-4.204354	5.040351	0.000000
16	1	0	-1.953848	6.089137	0.000000
17	6	0	-1.147797	-1.435139	0.000000
18	1	0	-1.949532	-2.158543	0.000000
19	6	0	0.932994	-0.449375	0.000000
20	6	0	0.224951	-1.676057	0.000000
21	6	0	2.376955	-0.721581	0.000000
22	1	0	3.174737	0.006155	0.000000
23	6	0	1.207335	-2.734491	0.000000
24	6	0	2.516539	-2.102423	0.000000
25	6	0	1.107823	-4.118029	0.000000
26	1	0	0.138103	-4.601536	0.000000
27	6	0	3.681965	-2.914920	0.000000
28	1	0	4.662812	-2.453849	0.000000
29	6	0	2.267734	-4.880296	0.000000
30	1	0	2.195709	-5.961350	0.000000
31	6	0	3.547049	-4.277879	0.000000
32	1	0	4.426890	-4.909586	0.000000
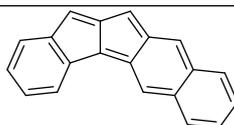
	S$_0$							T$_1$				

E = -769.0241569 a.u.   E = -769.0449047 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.276994	0.000000	1	6	0	0.000000	0.315113	0.000000
2	6	0	1.407427	0.440211	0.000000	2	6	0	1.359157	0.467583	0.000000
3	6	0	1.957229	1.696891	0.000000	3	6	0	1.928446	1.772759	0.000000
4	6	0	1.111604	2.893590	0.000000	4	6	0	1.075076	2.911852	0.000000
5	6	0	-0.250685	2.776864	0.000000	5	6	0	-0.340126	2.737314	0.000000
6	6	0	-0.860000	1.492569	0.000000	6	6	0	-0.875781	1.481543	0.000000
7	1	0	4.017938	1.008744	0.000000	7	1	0	3.973230	1.096676	0.000000
8	1	0	2.056921	-0.427368	0.000000	8	1	0	2.020684	-0.391322	0.000000
9	6	0	3.386802	1.890262	0.000000	9	6	0	3.326316	1.967059	0.000000
10	6	0	1.757391	4.184624	0.000000	10	6	0	1.659741	4.195826	0.000000
11	1	0	-0.870296	3.667256	0.000000	11	1	0	-0.976205	3.615929	0.000000
12	6	0	3.099937	4.300209	0.000000	12	6	0	3.022402	4.353640	0.000000
13	6	0	3.931526	3.124015	0.000000	13	6	0	3.865345	3.227927	0.000000
14	1	0	1.126256	5.066391	0.000000	14	1	0	1.010073	5.064038	0.000000
15	1	0	3.567147	5.277407	0.000000	15	1	0	3.452995	5.347729	0.000000
16	1	0	5.008622	3.242403	0.000000	16	1	0	4.940464	3.359941	0.000000
17	6	0	-2.181158	1.125380	0.000000	17	6	0	-2.248105	1.030962	0.000000
18	1	0	-3.036794	1.784142	0.000000	18	1	0	-3.115606	1.674564	0.000000
19	6	0	-0.834973	-0.812014	0.000000	19	6	0	-0.858625	-0.827844	0.000000
20	6	0	-2.194631	-0.325693	0.000000	20	6	0	-2.225895	-0.373374	0.000000
21	6	0	-0.888930	-2.270594	0.000000	21	6	0	-0.856654	-2.270096	0.000000
22	6	0	-3.057343	-1.374610	0.000000	22	6	0	-3.072188	-1.488731	0.000000
23	6	0	-2.272148	-2.616092	0.000000	23	6	0	-2.228067	-2.673204	0.000000
24	1	0	-4.139629	-1.335965	0.000000	24	1	0	-4.152761	-1.494806	0.000000
25	6	0	0.058765	-3.269787	0.000000	25	6	0	0.150381	-3.218903	0.000000
26	1	0	1.117066	-3.038891	0.000000	26	1	0	1.192967	-2.924580	0.000000
27	6	0	-2.680009	-3.931333	0.000000	27	6	0	-2.554060	-4.017459	0.000000
28	1	0	-3.733898	-4.186489	0.000000	28	1	0	-3.590103	-4.336145	0.000000
29	6	0	-1.706955	-4.939988	0.000000	29	6	0	-1.526639	-4.964480	0.000000
30	1	0	-2.007895	-5.980154	0.000000	30	1	0	-1.773079	-6.019439	0.000000
31	6	0	-0.364616	-4.608306	0.000000	31	6	0	-0.195305	-4.572295	0.000000
32	1	0	0.379171	-5.396623	0.000000	32	1	0	0.584827	-5.323728	0.000000
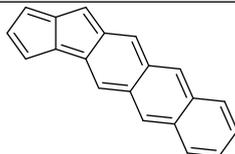
	S$_0$					T$_1$			
	E = -769.055359 a.u.					E = -769.0196408 a.u.			

Center Number	Atomic Number	Atomic Type	X	Y	Z	Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	1.640394	-1.003507	0.000000	1	6	0	1.617384	-1.062575	0.000000
2	6	0	1.367695	0.317330	0.000000	2	6	0	1.350652	0.280590	0.000000
3	6	0	0.000000	0.771755	0.000000	3	6	0	0.000000	0.741694	0.000000
4	6	0	-1.062599	-0.195184	0.000000	4	6	0	-1.074092	-0.219003	0.000000
5	6	0	-0.733708	-1.597060	0.000000	5	6	0	-0.771286	-1.621122	0.000000
6	6	0	0.559857	-1.982383	0.000000	6	6	0	0.520714	-2.046875	0.000000
7	1	0	0.482875	2.851591	0.000000	7	1	0	0.508615	2.819110	0.000000
8	1	0	2.159508	1.058098	0.000000	8	1	0	2.153570	1.009597	0.000000
9	6	0	-0.317393	2.118678	0.000000	9	6	0	-0.302312	2.097919	0.000000
10	6	0	-2.375354	0.242325	0.000000	10	6	0	-2.381054	0.242542	0.000000
11	1	0	-1.540240	-2.322416	0.000000	11	1	0	-1.593330	-2.328634	0.000000
12	6	0	-2.699812	1.605712	0.000000	12	6	0	-2.686289	1.609089	0.000000
13	6	0	-1.645824	2.566185	0.000000	13	6	0	-1.621310	2.560563	0.000000
14	1	0	-3.177743	-0.488373	0.000000	14	1	0	-3.194312	-0.475814	0.000000
15	6	0	1.157353	-3.326257	0.000000	15	6	0	1.094804	-3.368069	0.000000
16	1	0	0.580170	-4.242029	0.000000	16	1	0	0.535050	-4.291484	0.000000
17	6	0	2.876168	-1.782314	0.000000	17	6	0	2.821455	-1.807862	0.000000
18	6	0	2.498578	-3.203433	0.000000	18	6	0	2.492473	-3.210702	0.000000
19	6	0	4.222248	-1.703564	0.000000	19	6	0	4.265474	-1.673941	0.000000
20	1	0	4.839434	-0.816251	0.000000	20	1	0	4.828533	-0.752723	0.000000
21	6	0	3.729333	-3.978454	0.000000	21	6	0	3.697362	-3.917373	0.000000
22	6	0	4.745552	-3.083650	0.000000	22	6	0	4.779950	-2.934557	0.000000
23	1	0	3.813251	-5.054417	0.000000	23	1	0	3.833115	-4.989484	0.000000
24	1	0	5.799306	-3.328176	0.000000	24	1	0	5.830835	-3.187544	0.000000
25	6	0	-4.046366	2.065203	0.000000	25	6	0	-4.027373	2.086377	0.000000
26	1	0	-4.845570	1.332370	0.000000	26	1	0	-4.835676	1.363736	0.000000
27	6	0	-1.980451	3.949172	0.000000	27	6	0	-1.939866	3.948695	0.000000
28	1	0	-1.177734	4.678117	0.000000	28	1	0	-1.128163	4.667653	0.000000
29	6	0	-3.281200	4.353174	0.000000	29	6	0	-3.234888	4.367620	0.000000
30	1	0	-3.522885	5.409260	0.000000	30	1	0	-3.465606	5.426035	0.000000
31	6	0	-4.329701	3.397419	0.000000	31	6	0	-4.294000	3.421695	0.000000
32	1	0	-5.358992	3.735343	0.000000	32	1	0	-5.319417	3.771336	0.000000
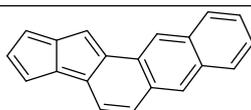
	S$_0$					T$_1$			
	E = -769.0434537 a.u.					E = -769.021512 a.u.			

Center Number	Atomic Number	Atomic Type	X	Y	Z	Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.948878	-2.007808	0.000000	1	6	0	0.668910	-2.143315	0.000000
2	6	0	-0.150479	-1.167247	0.000000	2	6	0	-0.356258	-1.140074	0.000000
3	6	0	0.000000	0.243628	0.000000	3	6	0	0.000000	0.249398	0.000000
4	6	0	1.342827	0.762300	0.000000	4	6	0	1.399703	0.582370	0.000000
5	6	0	2.444955	-0.141567	0.000000	5	6	0	2.389219	-0.469159	0.000000
6	6	0	2.260577	-1.494697	0.000000	6	6	0	2.041280	-1.779210	0.000000
7	1	0	-2.087025	0.760115	0.000000	7	1	0	-1.995011	1.023723	0.000000
8	6	0	-1.071374	1.138946	0.000000	8	6	0	-0.939029	1.268029	0.000000
9	6	0	1.533011	2.143871	0.000000	9	6	0	1.770661	1.912640	0.000000
10	1	0	3.446722	0.272800	0.000000	10	1	0	3.433318	-0.178521	0.000000
11	6	0	0.463760	3.032561	0.000000	11	6	0	0.823194	2.949057	0.000000
12	6	0	-0.873008	2.515151	0.000000	12	6	0	-0.563252	2.618307	0.000000
13	1	0	3.111047	-2.165899	0.000000	13	1	0	2.801391	-2.551323	0.000000

S81

14	6	0	-1.390650	-1.989846	0.000000
15	1	0	-2.395152	-1.588470	0.000000
16	6	0	0.426506	-3.382764	0.000000
17	6	0	-1.032408	-3.285318	0.000000
18	6	0	-1.559720	-4.654664	0.000000
19	1	0	-2.600316	-4.942089	0.000000
20	6	0	0.765199	-4.682996	0.000000
21	1	0	1.756948	-5.114878	0.000000
22	6	0	-0.494620	-5.479431	0.000000
23	1	0	-0.525468	-6.560046	0.000000
24	1	0	2.545129	2.535526	0.000000
25	6	0	0.650839	4.449210	0.000000
26	1	0	1.663628	4.836606	0.000000
27	6	0	-1.962551	3.440625	0.000000
28	1	0	-2.973757	3.049051	0.000000
29	6	0	-1.741253	4.779886	0.000000
30	1	0	-2.576951	5.469415	0.000000
31	6	0	-0.411874	5.293814	0.000000
32	1	0	-0.256494	6.365939	0.000000

14	6	0	-1.641338	-1.757657	0.000000
15	1	0	-2.590770	-1.243958	0.000000
16	6	0	0.016949	-3.392129	0.000000
17	6	0	-1.434277	-3.139429	0.000000
18	6	0	-2.078954	-4.375795	0.000000
19	1	0	-3.141330	-4.567959	0.000000
20	6	0	0.216098	-4.779412	0.000000
21	1	0	1.155242	-5.311879	0.000000
22	6	0	-1.058251	-5.369302	0.000000
23	1	0	-1.242371	-6.435592	0.000000
24	1	0	2.825146	2.168542	0.000000
25	6	0	1.199121	4.319297	0.000000
26	1	0	2.254101	4.569576	0.000000
27	6	0	-1.520412	3.670186	0.000000
28	1	0	-2.574132	3.414530	0.000000
29	6	0	-1.124388	4.973953	0.000000
30	1	0	-1.861818	5.767451	0.000000
31	6	0	0.254695	5.302531	0.000000
32	1	0	0.554210	6.343689	0.000000
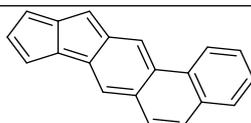
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	E = -769.0604072 a.u.			E = -769.0268033 a.u.	

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.305587	-1.860002	0.000000
2	6	0	1.412788	-1.072389	0.000000
3	6	0	1.277538	0.344927	0.000000
4	6	0	0.000000	0.942066	0.000000
5	6	0	-1.144140	0.095799	0.000000
6	6	0	-0.994219	-1.257989	0.000000
7	1	0	3.414438	0.686798	0.000000
8	1	0	2.409057	-1.500347	0.000000
9	6	0	2.443614	1.169466	0.000000
10	6	0	-0.104724	2.387016	0.000000
11	1	0	-2.138587	0.521606	0.000000
12	6	0	1.076773	3.166032	0.000000
13	6	0	2.349687	2.518105	0.000000
14	6	0	-2.008546	-2.333133	0.000000
15	1	0	-3.076596	-2.156695	0.000000
16	6	0	0.079996	-3.308152	0.000000
17	6	0	-1.372992	-3.518845	0.000000
18	6	0	0.682043	-4.511889	0.000000
19	1	0	1.741167	-4.728951	0.000000
20	6	0	-1.601324	-4.960558	0.000000
21	6	0	-0.382153	-5.542871	0.000000
22	1	0	-2.558089	-5.460134	0.000000
23	1	0	-0.190076	-6.607171	0.000000
24	6	0	0.986583	4.573474	0.000000
25	6	0	-1.342030	3.066900	0.000000
26	1	0	-2.267120	2.507149	0.000000
27	6	0	-1.405512	4.437554	0.000000
28	1	0	-2.370214	4.930702	0.000000
29	6	0	-0.229636	5.203960	0.000000
30	1	0	-0.286569	6.285682	0.000000
31	1	0	3.242611	3.132943	0.000000
32	1	0	1.903975	5.151596	0.000000

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	0.204300	-1.875938	0.000000
2	6	0	1.351166	-1.115480	0.000000
3	6	0	1.267243	0.290284	0.000000
4	6	0	0.000000	0.932664	0.000000
5	6	0	-1.170956	0.141404	0.000000
6	6	0	-1.090523	-1.230068	0.000000
7	1	0	3.415948	0.560036	0.000000
8	1	0	2.329274	-1.583870	0.000000
9	6	0	2.463227	1.077589	0.000000
10	6	0	-0.046483	2.385210	0.000000
11	1	0	-2.145469	0.610254	0.000000
12	6	0	1.162955	3.118702	0.000000
13	6	0	2.416844	2.425663	0.000000
14	6	0	-2.122758	-2.241569	0.000000
15	1	0	-3.185414	-2.048787	0.000000
16	6	0	-0.041120	-3.278920	0.000000
17	6	0	-1.476939	-3.487335	0.000000
18	6	0	0.608633	-4.561116	0.000000
19	1	0	1.671544	-4.749514	0.000000
20	6	0	-1.693646	-4.862043	0.000000
21	6	0	-0.380257	-5.505039	0.000000
22	1	0	-2.639563	-5.383858	0.000000
23	1	0	-0.227988	-6.575456	0.000000
24	6	0	1.125111	4.526288	0.000000
25	6	0	-1.256448	3.109187	0.000000
26	1	0	-2.201097	2.583594	0.000000
27	6	0	-1.270511	4.482651	0.000000
28	1	0	-2.216421	5.010654	0.000000
29	6	0	-0.068146	5.202894	0.000000
30	1	0	-0.083497	6.286005	0.000000
31	1	0	3.329502	3.010440	0.000000
32	1	0	2.063030	5.070325	0.000000

	S$_0$	
	E = -769.054772 a.u.	

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.525325	-1.265177	0.000000
2	6	0	1.296361	0.116909	0.000000
3	6	0	0.000000	0.640330	0.000000
4	6	0	-1.097764	-0.268590	0.000000
5	6	0	-0.832755	-1.645263	0.000000
6	6	0	0.458116	-2.148011	0.000000
7	1	0	0.590678	2.735285	0.000000
8	6	0	-0.251246	2.054605	0.000000
9	6	0	-2.454899	0.265373	0.000000
10	1	0	-1.653128	-2.349159	0.000000
11	6	0	-2.646380	1.664231	0.000000
12	6	0	-1.507793	2.538754	0.000000
13	6	0	-3.950025	2.192975	0.000000
14	6	0	-3.599500	-0.554477	0.000000
15	1	0	-3.495046	-1.630632	0.000000
16	6	0	-4.865972	-0.018792	0.000000
17	1	0	-5.726780	-0.676654	0.000000
18	6	0	-5.048225	1.369320	0.000000
19	1	0	-6.047444	1.787402	0.000000
20	1	0	-1.684028	3.608587	0.000000
21	1	0	-4.073467	3.270321	0.000000
22	1	0	0.622315	-3.218880	0.000000
23	6	0	2.609071	0.815836	0.000000
24	1	0	2.735664	1.889868	0.000000
25	6	0	2.982955	-1.448569	0.000000
26	6	0	3.581003	-0.112688	0.000000
27	6	0	5.035487	-0.287517	0.000000
28	1	0	5.777070	0.496877	0.000000
29	6	0	3.973657	-2.356890	0.000000
30	1	0	3.891555	-3.435254	0.000000
31	6	0	5.264042	-1.616284	0.000000
32	1	0	6.233861	-2.094209	0.000000

	T$_1$	
	E = -769.0267876 a.u.	

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.558267	-1.232952	0.000000
2	6	0	1.322838	0.172419	0.000000
3	6	0	0.000000	0.672670	0.000000
4	6	0	-1.076292	-0.246642	0.000000
5	6	0	-0.800177	-1.640999	0.000000
6	6	0	0.479593	-2.128780	0.000000
7	1	0	0.571790	2.766336	0.000000
8	6	0	-0.264305	2.078858	0.000000
9	6	0	-2.434504	0.264361	0.000000
10	1	0	-1.618696	-2.346006	0.000000
11	6	0	-2.648895	1.662768	0.000000
12	6	0	-1.528254	2.552005	0.000000
13	6	0	-3.963439	2.169447	0.000000
14	6	0	-3.569150	-0.574954	0.000000
15	1	0	-3.448432	-1.649028	0.000000
16	6	0	-4.841547	-0.059621	0.000000
17	1	0	-5.692531	-0.730048	0.000000
18	6	0	-5.045640	1.327856	0.000000
19	1	0	-6.051880	1.728884	0.000000
20	1	0	-1.717117	3.619479	0.000000
21	1	0	-4.104792	3.244476	0.000000
22	1	0	0.655891	-3.197840	0.000000
23	6	0	2.584009	0.873882	0.000000
24	1	0	2.713822	1.945217	0.000000
25	6	0	2.967140	-1.418187	0.000000
26	6	0	3.593639	-0.095537	0.000000
27	6	0	4.967889	-0.286507	0.000000
28	1	0	5.743797	0.464610	0.000000
29	6	0	3.990900	-2.400821	0.000000
30	1	0	3.868336	-3.473294	0.000000
31	6	0	5.192787	-1.720856	0.000000
32	1	0	6.170655	-2.183258	0.000000

Absolute energies and x, y, z coordinates of optimized structures in T₁ state (M06-2X)
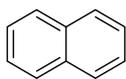
E = -385.7050592 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	2.479832	0.677590
2	6	0	0.000000	1.230483	1.397565
3	6	0	0.000000	0.000000	0.724572
4	6	0	0.000000	0.000000	-0.724572
5	6	0	0.000000	1.230483	-1.397565
6	6	0	0.000000	2.479832	-0.677590
7	1	0	0.000000	-1.237632	2.481194
8	1	0	0.000000	3.409425	1.233171
9	1	0	0.000000	1.237632	2.481194
10	6	0	0.000000	-1.230483	1.397565
11	6	0	0.000000	-1.230483	-1.397565
12	1	0	0.000000	1.237632	-2.481194
13	1	0	0.000000	3.409425	-1.233171
14	6	0	0.000000	-2.479832	-0.677590
15	6	0	0.000000	-2.479832	0.677590
16	1	0	0.000000	-1.237632	-2.481194
17	1	0	0.000000	-3.409425	-1.233171
18	1	0	0.000000	-3.409425	1.233171
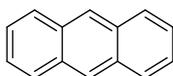
E = -539.3501165 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	-3.692385	0.688949
2	6	0	0.000000	-2.471221	1.390626
3	6	0	0.000000	-1.255841	0.716290
4	6	0	0.000000	-1.255841	-0.716290
5	6	0	0.000000	-2.471221	-1.390626
6	6	0	0.000000	-3.692385	-0.688949
7	6	0	0.000000	0.000000	1.406530
8	6	0	0.000000	0.000000	-1.406530
9	6	0	0.000000	1.255841	-0.716290
10	6	0	0.000000	1.255841	0.716290
11	6	0	0.000000	2.471221	1.390626
12	1	0	0.000000	2.472274	2.475290
13	6	0	0.000000	3.692385	0.688949
14	6	0	0.000000	3.692385	-0.688949
15	6	0	0.000000	2.471221	-1.390626
16	1	0	0.000000	0.000000	2.490807
17	1	0	0.000000	-4.626200	1.237735
18	1	0	0.000000	-2.472274	2.475290
19	1	0	0.000000	-2.472274	-2.475290
20	1	0	0.000000	-4.626200	-1.237735
21	1	0	0.000000	0.000000	-2.490807
22	1	0	0.000000	4.626200	1.237735
23	1	0	0.000000	4.626200	-1.237735
24	1	0	0.000000	2.472274	-2.475290
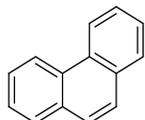
E = -539.3232805 a.u.

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Center     Atomic      Atomic          Coordinates (Angstroms)
Number     Number      Type          X         Y         Z
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   1         6          0      0.000000    3.582538   -0.311255
   2         6          0      0.000000    2.873159    0.872869
   3         6          0      0.000000    1.444442    0.883074
   4         6          0      0.000000    0.746665   -0.381916
   5         6          0      0.000000    1.490554   -1.540686
   6         6          0      0.000000    2.901024   -1.525495
   7         6          0      0.000000    0.739083    2.073021
   8         6          0      0.000000   -0.746665   -0.381916
   9         6          0      0.000000   -1.444442    0.883074
  10         6          0      0.000000   -0.739083    2.073021
  11         6          0      0.000000   -2.873159    0.872869
  12         1          0      0.000000   -3.392380    1.824850
  13         6          0      0.000000   -3.582538   -0.311255
  14         6          0      0.000000   -2.901024   -1.525495
  15         6          0      0.000000   -1.490554   -1.540686
  16         1          0      0.000000    1.269019    3.017089
  17         1          0      0.000000    4.665796   -0.294323
  18         1          0      0.000000    3.392380    1.824850
  19         1          0      0.000000    0.997419   -2.504249
  20         1          0      0.000000    3.445648   -2.461039
  21         1          0      0.000000   -1.269019    3.017089
  22         1          0      0.000000   -4.665796   -0.294323
  23         1          0      0.000000   -3.445648   -2.461039
  24         1          0      0.000000   -0.997419   -2.504249
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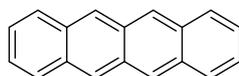

E = -692.979846 a.u.

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---------------------------------------------------------------------
Center     Atomic      Atomic          Coordinates (Angstroms)
Number     Number      Type          X         Y         Z
---------------------------------------------------------------------
   1         6          0      0.000000   -4.906511   -0.696350
   2         6          0      0.000000   -3.701406   -1.392241
   3         6          0      0.000000   -2.479317   -0.712140
   4         6          0      0.000000   -2.479317    0.712140
   5         6          0      0.000000   -3.701406    1.392241
   6         6          0      0.000000   -4.906511    0.696350
   7         6          0      0.000000   -1.223721   -1.403308
   8         6          0      0.000000   -1.223721    1.403308
   9         6          0      0.000000    0.000000    0.731127
  10         6          0      0.000000    0.000000   -0.731127
  11         6          0      0.000000    1.223721   -1.403308
  12         1          0      0.000000    1.229988   -2.488535
  13         6          0      0.000000    2.479317   -0.712140
  14         6          0      0.000000    2.479317    0.712140
  15         6          0      0.000000    1.223721    1.403308
  16         1          0      0.000000   -1.229988   -2.488535
  17         1          0      0.000000   -5.843434   -1.240021
  18         1          0      0.000000   -3.699731   -2.476997
  19         1          0      0.000000   -3.699731    2.476997
  20         1          0      0.000000   -5.843434    1.240021
  21         1          0      0.000000   -1.229988    2.488535
  22         1          0      0.000000    1.229988    2.488535
  23         6          0      0.000000    3.701406    1.392241
  24         1          0      0.000000    3.699731    2.476997
```

25	6	0	0.000000	3.701406	-1.392241
26	1	0	0.000000	3.699731	-2.476997
27	6	0	0.000000	4.906511	0.696350
28	1	0	0.000000	5.843434	1.240021
29	6	0	0.000000	4.906511	-0.696350
30	1	0	0.000000	5.843434	-1.240021
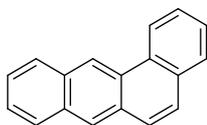
E = -692.9621699 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z

Coordinates (Angstroms)

1	6	0	-0.503860	-4.755940	0.000000
2	6	0	0.601162	-3.875908	0.000000
3	6	0	0.419081	-2.496785	0.000000
4	6	0	-0.913234	-1.968754	0.000000
5	6	0	-1.985013	-2.849605	0.000000
6	6	0	-1.781151	-4.249879	0.000000
7	6	0	1.506417	-1.577041	0.000000
8	6	0	-1.096821	-0.546366	0.000000
9	6	0	0.000000	0.379393	0.000000
10	6	0	1.309965	-0.144202	0.000000
11	6	0	2.414773	0.721130	0.000000
12	1	0	3.412244	0.295095	0.000000
13	6	0	2.249664	2.091967	0.000000
14	6	0	0.961630	2.654464	0.000000
15	6	0	-0.185131	1.794260	0.000000
16	1	0	2.521030	-1.959003	0.000000
17	1	0	-0.336256	-5.825954	0.000000
18	1	0	1.609544	-4.275115	0.000000
19	1	0	-2.995162	-2.454508	0.000000
20	1	0	-2.636061	-4.914810	0.000000
21	1	0	-2.115145	-0.183614	0.000000
22	1	0	3.112286	2.748868	0.000000
23	6	0	0.778456	4.065111	0.000000
24	1	0	1.659846	4.697656	0.000000
25	6	0	-1.471550	2.407610	0.000000
26	1	0	-2.362553	1.794305	0.000000
27	6	0	-1.610942	3.767502	0.000000
28	1	0	-2.601938	4.205623	0.000000
29	6	0	-0.471479	4.613445	0.000000
30	1	0	-0.599640	5.689058	0.000000
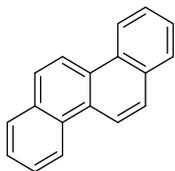
E = -692.9490924 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z

Coordinates (Angstroms)

1	6	0	0.643420	2.521618	0.000000
2	6	0	-0.612564	1.855623	0.000000
3	6	0	-0.643420	0.369677	0.000000
4	6	0	0.643420	-0.369677	0.000000
5	6	0	1.810275	0.333826	0.000000
6	6	0	1.843845	1.754705	0.000000

Center Number	Atomic Number	Atomic Type	X	Y	Z
7	1	0	-2.760655	0.183300	0.000000
8	6	0	-1.810275	-0.333826	0.000000
9	6	0	0.612564	-1.855623	0.000000
10	1	0	2.760655	-0.183300	0.000000
11	1	0	2.796253	2.269838	0.000000
12	6	0	-0.643420	-2.521618	0.000000
13	6	0	-1.843845	-1.754705	0.000000
14	1	0	-2.796253	-2.269838	0.000000
15	6	0	1.764991	-2.630918	0.000000
16	1	0	2.740058	-2.161653	0.000000
17	6	0	-0.684183	-3.925035	0.000000
18	1	0	-1.650463	-4.417787	0.000000
19	6	0	1.710206	-4.029399	0.000000
20	1	0	2.631108	-4.599629	0.000000
21	6	0	0.483867	-4.677181	0.000000
22	1	0	0.434359	-5.759306	0.000000
23	6	0	0.684183	3.925035	0.000000
24	1	0	1.650463	4.417787	0.000000
25	6	0	-1.764991	2.630918	0.000000
26	1	0	-2.740058	2.161653	0.000000
27	6	0	-1.710206	4.029399	0.000000
28	1	0	-2.631108	4.599629	0.000000
29	6	0	-0.483867	4.677181	0.000000
30	1	0	-0.434359	5.759306	0.000000
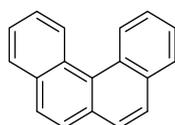
E = -692.9266948 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-3.928749	-1.607153	0.000000
2	6	0	-3.781557	-0.211491	0.000000
3	6	0	-2.526805	0.401604	0.000000
4	6	0	-1.313400	-0.385003	0.000000
5	6	0	-1.514307	-1.761774	0.000000
6	6	0	-2.795613	-2.372285	0.000000
7	6	0	-2.479765	1.820817	0.000000
8	6	0	0.000000	0.318240	0.000000
9	6	0	-0.057702	1.818828	0.000000
10	6	0	-1.238924	2.495809	0.000000
11	6	0	1.151767	2.599248	0.000000
12	1	0	1.046930	3.678534	0.000000
13	6	0	2.357600	2.021044	0.000000
14	6	0	2.486693	0.574047	0.000000
15	6	0	1.321288	-0.276627	0.000000
16	1	0	-3.408463	2.376981	0.000000
17	1	0	-4.914231	-2.056177	0.000000
18	1	0	-4.659889	0.424435	0.000000
19	1	0	-0.700842	-2.454380	0.000000
20	1	0	-2.852480	-3.453776	0.000000
21	1	0	-1.220631	3.579672	0.000000
22	1	0	3.266139	2.612325	0.000000
23	6	0	1.617730	-1.665482	0.000000
24	1	0	0.847219	-2.405283	0.000000
25	6	0	2.912183	-2.172504	0.000000
26	1	0	3.050310	-3.247139	0.000000
27	6	0	3.770111	0.048548	0.000000
28	1	0	4.605763	0.739909	0.000000
29	6	0	4.006580	-1.326034	0.000000
30	1	0	5.017391	-1.714097	0.000000
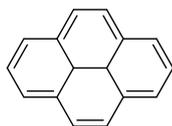
E = -615.5708457 a.u.

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---------------------------------------------------------------------
Center    Atomic    Atomic         Coordinates (Angstroms)
Number    Number    Type        X         Y          Z
---------------------------------------------------------------------
   1        6        0       0.000000   0.000000   3.547481
   2        6        0       0.000000   1.206022   2.865586
   3        6        0       0.000000   1.237367   1.418578
   4        6        0       0.000000   0.000000   0.706449
   5        6        0       0.000000  -1.237367   1.418578
   6        6        0       0.000000  -1.206022   2.865586
   7        6        0       0.000000   2.426013   0.704021
   8        6        0       0.000000   0.000000  -0.706449
   9        6        0       0.000000   1.237367  -1.418578
  10        6        0       0.000000   2.426013  -0.704021
  11        6        0       0.000000   1.206022  -2.865586
  12        1        0       0.000000   2.146180  -3.403976
  13        6        0       0.000000   0.000000  -3.547481
  14        6        0       0.000000  -1.206022  -2.865586
  15        6        0       0.000000  -1.237367  -1.418578
  16        6        0       0.000000  -2.426013  -0.704021
  17        6        0       0.000000  -2.426013   0.704021
  18        1        0       0.000000  -3.368080   1.241103
  19        1        0       0.000000  -3.368080  -1.241103
  20        1        0       0.000000   3.368080   1.241103
  21        1        0       0.000000   0.000000   4.631169
  22        1        0       0.000000   2.146180   3.403976
  23        1        0       0.000000  -2.146180   3.403976
  24        1        0       0.000000   3.368080  -1.241103
  25        1        0       0.000000   0.000000  -4.631169
  26        1        0       0.000000  -2.146180  -3.403976
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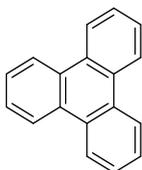

E = -692.9302039 a.u.

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---------------------------------------------------------------------
Center    Atomic    Atomic         Coordinates (Angstroms)
Number    Number    Type        X         Y          Z
---------------------------------------------------------------------
   1        6        0       0.094236   2.510112  -1.381457
   2        6        0      -0.010827   1.290816  -0.704715
   3        6        0      -0.081613   0.011946  -1.433466
   4        6        0      -0.373149  -0.063685  -2.769137
   5        6        0      -0.010827   1.290816   0.704715
   6        6        0       0.174317  -1.231368  -0.684690
   7        6        0       0.174317  -1.231368   0.684690
   8        6        0      -0.081613   0.011946   1.433466
   9        6        0       0.321766  -2.458512   1.475523
  10        6        0       0.321766  -2.458512  -1.475523
  11        6        0       0.055372  -2.471643  -2.810870
  12        6        0      -0.336801  -1.289229  -3.477941
  13        1        0      -0.575978  -1.308515  -4.532907
  14        1        0       0.145188  -3.396404  -3.368679
  15        6        0       0.165259   3.714373  -0.694959
  16        6        0       0.165259   3.714373   0.694959
  17        6        0       0.094236   2.510112   1.381457
  18        1        0       0.243699   4.645241  -1.243527
```

19	1	0	0.243699	4.645241	1.243527
20	6	0	-0.373149	-0.063685	2.769137
21	6	0	0.055372	-2.471643	2.810870
22	1	0	0.145188	-3.396404	3.368679
23	6	0	-0.336801	-1.289229	3.477941
24	1	0	-0.575978	-1.308515	4.532907
25	1	0	0.630717	-3.371974	0.988992
26	1	0	-0.638022	0.833043	3.315291
27	1	0	0.143027	2.521750	2.462686
28	1	0	0.143027	2.521750	-2.462686
29	1	0	0.630717	-3.371974	-0.988992
30	1	0	-0.638022	0.833043	-3.315291
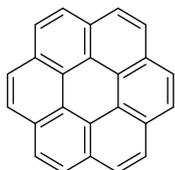
E = -921.6288275 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z
			Coordinates (Angstroms)		
1	6	0	0.000000	1.243126	-3.549228
2	6	0	0.000000	0.000000	-2.868678
3	6	0	0.000000	0.000000	-1.415605
4	6	0	0.000000	1.219496	-0.711667
5	6	0	0.000000	2.463616	-1.421941
6	6	0	0.000000	2.426253	-2.871478
7	6	0	0.000000	-1.219496	-0.711667
8	6	0	0.000000	1.219496	0.711667
9	6	0	0.000000	0.000000	1.415605
10	6	0	0.000000	-1.219496	0.711667
11	6	0	0.000000	0.000000	2.868678
12	6	0	0.000000	1.243126	3.549228
13	6	0	0.000000	2.426253	2.871478
14	6	0	0.000000	2.463616	1.421941
15	6	0	0.000000	3.646063	0.710489
16	6	0	0.000000	3.646063	-0.710489
17	1	0	0.000000	4.589495	-1.244871
18	1	0	0.000000	4.589495	1.244871
19	1	0	0.000000	1.237268	-4.634070
20	1	0	0.000000	3.368590	-3.407433
21	1	0	0.000000	1.237268	4.634070
22	1	0	0.000000	3.368590	3.407433
23	6	0	0.000000	-1.243126	-3.549228
24	6	0	0.000000	-2.426253	-2.871478
25	6	0	0.000000	-2.463616	-1.421941
26	1	0	0.000000	-1.237268	-4.634070
27	1	0	0.000000	-3.368590	-3.407433
28	6	0	0.000000	-3.646063	-0.710489
29	6	0	0.000000	-3.646063	0.710489
30	6	0	0.000000	-2.463616	1.421941
31	1	0	0.000000	-4.589495	-1.244871
32	1	0	0.000000	-4.589495	1.244871
33	6	0	0.000000	-1.243126	3.549228
34	1	0	0.000000	-1.237268	4.634070
35	6	0	0.000000	-2.426253	2.871478
36	1	0	0.000000	-3.368590	3.407433
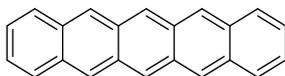
E = -846.6020455 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.699560	-0.711482
2	6	0	0.000000	2.451781	-1.399922
3	6	0	0.000000	1.243045	-0.728255
4	6	0	0.000000	1.243045	0.728255
5	6	0	0.000000	2.451781	1.399922
6	6	0	0.000000	3.699560	0.711482
7	6	0	0.000000	0.000000	-1.408233
8	6	0	0.000000	0.000000	1.408233
9	6	0	0.000000	-1.243045	0.728255
10	6	0	0.000000	-1.243045	-0.728255
11	6	0	0.000000	-2.451781	-1.399922
12	1	0	0.000000	-2.456849	-2.485585
13	6	0	0.000000	-3.699560	-0.711482
14	6	0	0.000000	-3.699560	0.711482
15	6	0	0.000000	-2.451781	1.399922
16	1	0	0.000000	0.000000	-2.493233
17	1	0	0.000000	2.456849	-2.485585
18	1	0	0.000000	2.456849	2.485585
19	1	0	0.000000	0.000000	2.493233
20	1	0	0.000000	-2.456849	2.485585
21	6	0	0.000000	-4.930964	1.395185
22	1	0	0.000000	-4.927505	2.479910
23	6	0	0.000000	-4.930964	-1.395185
24	1	0	0.000000	-4.927505	-2.479910
25	6	0	0.000000	-6.124125	0.702182
26	1	0	0.000000	-7.063776	1.241233
27	6	0	0.000000	-6.124125	-0.702182
28	1	0	0.000000	-7.063776	-1.241233
29	6	0	0.000000	4.930964	1.395185
30	1	0	0.000000	4.927505	2.479910
31	6	0	0.000000	6.124125	0.702182
32	1	0	0.000000	7.063776	1.241233
33	6	0	0.000000	4.930964	-1.395185
34	1	0	0.000000	4.927505	-2.479910
35	6	0	0.000000	6.124125	-0.702182
36	1	0	0.000000	7.063776	-1.241233
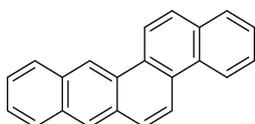
E = -846.5839613 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.533515	-1.681623	0.000000
2	6	0	-0.430247	-0.615756	0.000000
3	6	0	0.000000	0.737404	0.000000
4	6	0	1.393351	1.025067	0.000000
5	6	0	2.307198	-0.025846	0.000000
6	6	0	1.887344	-1.353197	0.000000
7	6	0	-0.904430	1.845888	0.000000
8	6	0	1.842210	2.390813	0.000000
9	6	0	0.937651	3.493204	0.000000
10	6	0	-0.465496	3.212530	0.000000
11	6	0	-1.363307	4.271787	0.000000
12	1	0	-2.427829	4.063392	0.000000
13	6	0	-0.912597	5.608991	0.000000
14	6	0	0.437657	5.878224	0.000000
15	6	0	1.365075	4.817277	0.000000
16	1	0	-1.972473	1.681576	0.000000
17	1	0	3.368157	0.199574	0.000000
18	1	0	2.640775	-2.128440	0.000000

19	1	0	2.909105	2.583983	0.000000
20	1	0	-1.632873	6.417800	0.000000
21	1	0	0.793434	6.901267	0.000000
22	1	0	2.428965	5.028508	0.000000
23	6	0	-1.827326	-0.959931	0.000000
24	1	0	-2.570889	-0.175621	0.000000
25	6	0	0.074718	-3.069416	0.000000
26	6	0	-1.312185	-3.339745	0.000000
27	6	0	-2.244221	-2.244681	0.000000
28	1	0	-3.304370	-2.474607	0.000000
29	6	0	0.958069	-4.167287	0.000000
30	1	0	2.027658	-4.007334	0.000000
31	6	0	-1.772860	-4.669158	0.000000
32	1	0	-2.842736	-4.848563	0.000000
33	6	0	-0.887463	-5.724163	0.000000
34	1	0	-1.250551	-6.744728	0.000000
35	6	0	0.489943	-5.465093	0.000000
36	1	0	1.194038	-6.288545	0.000000
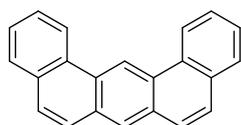
E = -846.5728636 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	0.000000	-3.736168	0.302501
2	6	0	0.000000	-2.511918	-0.450841
3	6	0	0.000000	-1.266982	0.238666
4	6	0	0.000000	-1.262419	1.648545
5	6	0	0.000000	-2.469905	2.360937
6	6	0	0.000000	-3.687062	1.703452
7	6	0	0.000000	0.000000	-0.446374
8	6	0	0.000000	0.000000	2.342811
9	6	0	0.000000	1.262419	1.648545
10	6	0	0.000000	1.266982	0.238666
11	6	0	0.000000	2.511918	-0.450841
12	6	0	0.000000	3.736168	0.302501
13	6	0	0.000000	3.687062	1.703452
14	6	0	0.000000	2.469905	2.360937
15	1	0	0.000000	0.000000	-1.523212
16	1	0	0.000000	-2.437725	3.445037
17	1	0	0.000000	-4.614370	2.265216
18	1	0	0.000000	0.000000	3.426403
19	1	0	0.000000	4.614370	2.265216
20	1	0	0.000000	2.437725	3.445037
21	6	0	0.000000	-2.614856	-1.874700
22	1	0	0.000000	-1.719872	-2.481974
23	6	0	0.000000	-4.982720	-0.385697
24	6	0	0.000000	-5.035062	-1.748009
25	6	0	0.000000	-3.828916	-2.499647
26	1	0	0.000000	-3.875918	-3.582149
27	1	0	0.000000	-5.988384	-2.262179
28	1	0	0.000000	-5.893369	0.203891
29	6	0	0.000000	2.614856	-1.874700
30	1	0	0.000000	1.719872	-2.481974
31	6	0	0.000000	4.982720	-0.385697
32	1	0	0.000000	5.893369	0.203891
33	6	0	0.000000	5.035062	-1.748009
34	1	0	0.000000	5.988384	-2.262179
35	6	0	0.000000	3.828916	-2.499647
36	1	0	0.000000	3.875918	-3.582149
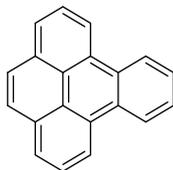
E = -769.1801691 a.u.

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-----------------------------------------------------------------
Center     Atomic      Atomic            Coordinates (Angstroms)
Number     Number      Type         X          Y          Z
-----------------------------------------------------------------
   1         6          0        0.000000   3.551789  -0.905495
   2         6          0        0.000000   2.861467  -2.102657
   3         6          0        0.000000   1.421271  -2.113772
   4         6          0        0.000000   0.715922  -0.854017
   5         6          0        0.000000   1.431216   0.354418
   6         6          0        0.000000   2.876723   0.303482
   7         6          0        0.000000   0.714049  -3.295604
   8         6          0        0.000000  -0.715922  -0.854017
   9         6          0        0.000000  -1.421271  -2.113772
  10         6          0        0.000000  -0.714049  -3.295604
  11         6          0        0.000000  -2.861467  -2.102657
  12         1          0        0.000000  -3.387377  -3.049923
  13         6          0        0.000000  -3.551789  -0.905495
  14         6          0        0.000000  -2.876723   0.303482
  15         6          0        0.000000  -1.431216   0.354418
  16         6          0        0.000000  -0.715637   1.593247
  17         6          0        0.000000   0.715637   1.593247
  18         1          0        0.000000   1.250006  -4.237755
  19         1          0        0.000000   4.635356  -0.908830
  20         1          0        0.000000   3.387377  -3.049923
  21         1          0        0.000000   3.452832   1.216052
  22         1          0        0.000000  -1.250006  -4.237755
  23         1          0        0.000000  -4.635356  -0.908830
  24         1          0        0.000000  -3.452832   1.216052
  25         6          0        0.000000  -1.389252   2.846033
  26         1          0        0.000000  -2.469196   2.875760
  27         6          0        0.000000   1.389252   2.846033
  28         1          0        0.000000   2.469196   2.875760
  29         6          0        0.000000   0.706195   4.030419
  30         1          0        0.000000   1.248227   4.968381
  31         6          0        0.000000  -0.706195   4.030419
  32         1          0        0.000000  -1.248227   4.968381
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E = -308.2480187 a.u.

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-----------------------------------------------------------------
Center     Atomic      Atomic            Coordinates (Angstroms)
Number     Number      Type         X          Y          Z
-----------------------------------------------------------------
   1         6          0        0.000000   1.460304  -0.630707
   2         6          0        0.000000   0.728720   0.558932
   3         6          0        0.000000  -0.728720   0.558932
   4         6          0        0.000000  -1.460304  -0.630707
   5         6          0        0.000000  -0.712061  -1.798795
   6         6          0        0.000000   0.712061  -1.798795
   7         1          0        0.000000   2.542901  -0.656223
   8         1          0        0.000000  -2.542901  -0.656223
   9         1          0        0.000000  -1.221831  -2.755032
  10         1          0        0.000000   1.221831  -2.755032
  11         6          0        0.000000  -0.738780   1.981326
  12         1          0        0.000000  -1.499331   2.746725
  13         6          0        0.000000   0.738780   1.981326
  14         1          0        0.000000   1.499331   2.746725
-----------------------------------------------------------------
```
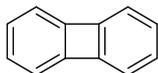
E = -461.8592831 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number      Type        X          Y          Z
---------------------------------------------------------------
    1         6           0       0.000000   1.468427   1.910457
    2         6           0       0.000000   0.738131   0.711731
    3         6           0       0.000000  -0.738131   0.711731
    4         6           0       0.000000  -1.468427   1.910457
    5         6           0       0.000000  -0.722870   3.067791
    6         6           0       0.000000   0.722870   3.067791
    7         1           0       0.000000   2.551080   1.939169
    8         1           0       0.000000  -2.551080   1.939169
    9         1           0       0.000000  -1.227045   4.026811
   10         1           0       0.000000   1.227045   4.026811
   11         6           0       0.000000  -0.738131  -0.711731
   12         6           0       0.000000   0.738131  -0.711731
   13         6           0       0.000000  -1.468427  -1.910457
   14         1           0       0.000000  -2.551080  -1.939169
   15         6           0       0.000000   1.468427  -1.910457
   16         1           0       0.000000   2.551080  -1.939169
   17         6           0       0.000000   0.722870  -3.067791
   18         1           0       0.000000   1.227045  -4.026811
   19         6           0       0.000000  -0.722870  -3.067791
   20         1           0       0.000000  -1.227045  -4.026811
---------------------------------------------------------------
```
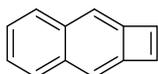

E = -461.8624356 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number      Type        X          Y          Z
---------------------------------------------------------------
    1         6           0       0.000000   0.710761  -3.016801
    2         6           0       0.000000   1.397732  -1.836598
    3         6           0       0.000000   0.725184  -0.580809
    4         6           0       0.000000  -0.725184  -0.580809
    5         6           0       0.000000  -1.397732  -1.836598
    6         6           0       0.000000  -0.710761  -3.016801
    7         1           0       0.000000   2.545952   0.596478
    8         1           0       0.000000   1.246607  -3.958320
    9         1           0       0.000000   2.482432  -1.834221
   10         6           0       0.000000   1.462372   0.624954
   11         6           0       0.000000  -1.462372   0.624954
   12         1           0       0.000000  -2.482432  -1.834221
   13         1           0       0.000000  -1.246607  -3.958320
   14         6           0       0.000000  -0.735906   1.798257
   15         6           0       0.000000   0.735906   1.798257
   16         1           0       0.000000  -2.545952   0.596478
   17         6           0       0.000000  -0.749334   3.213931
   18         1           0       0.000000  -1.510574   3.978458
   19         6           0       0.000000   0.749334   3.213931
   20         1           0       0.000000   1.510574   3.978458
---------------------------------------------------------------
```
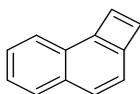

E = -461.8737081 a.u.

```
---------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number      Type        X          Y          Z
```

```
-----------------------------------------------------------------
   1      6      0     -2.672566    1.416706    0.000000
   2      6      0     -2.372647    0.066067    0.000000
   3      6      0     -1.042255   -0.381960    0.000000
   4      6      0      0.000000    0.596702    0.000000
   5      6      0     -0.324268    1.965429    0.000000
   6      6      0     -1.643937    2.370338    0.000000
   7      1      0     -1.588067   -2.479154    0.000000
   8      1      0     -3.706543    1.740177    0.000000
   9      1      0     -3.172989   -0.666496    0.000000
  10      6      0     -0.743073   -1.799340    0.000000
  11      6      0      1.314386    0.066494    0.000000
  12      1      0      0.477457    2.695392    0.000000
  13      1      0     -1.886773    3.426251    0.000000
  14      6      0      1.573215   -1.364037    0.000000
  15      6      0      0.541052   -2.304015    0.000000
  16      1      0      0.720966   -3.371992    0.000000
  17      6      0      2.983459   -1.098178    0.000000
  18      1      0      3.878623   -1.700910    0.000000
  19      6      0      2.711412    0.323655    0.000000
  20      1      0      3.328658    1.209562    0.000000
-----------------------------------------------------------------
```
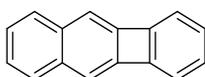

E = -615.4581372 a.u.

```
-----------------------------------------------------------------
Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number   Type          X        Y        Z
-----------------------------------------------------------------
   1      6      0      0.000000    0.701237   -4.292749
   2      6      0      0.000000    1.394056   -3.096044
   3      6      0      0.000000    0.730789   -1.851777
   4      6      0      0.000000   -0.730789   -1.851777
   5      6      0      0.000000   -1.394056   -3.096044
   6      6      0      0.000000   -0.701237   -4.292749
   7      1      0      0.000000    2.559359   -0.649657
   8      1      0      0.000000    1.242875   -5.230884
   9      1      0      0.000000    2.478269   -3.096087
  10      6      0      0.000000    1.478273   -0.632454
  11      6      0      0.000000   -1.478273   -0.632454
  12      1      0      0.000000   -2.478269   -3.096087
  13      1      0      0.000000   -1.242875   -5.230884
  14      6      0      0.000000   -0.722917    0.527481
  15      6      0      0.000000    0.722917    0.527481
  16      1      0      0.000000   -2.559359   -0.649657
  17      6      0      0.000000   -0.724011    1.973004
  18      6      0      0.000000    0.724011    1.973004
  19      6      0      0.000000   -1.475228    3.138387
  20      1      0      0.000000   -2.555123    3.158224
  21      6      0      0.000000    1.475228    3.138387
  22      1      0      0.000000    2.555123    3.158224
  23      6      0      0.000000    0.698997    4.323624
  24      1      0      0.000000    1.206220    5.281576
  25      6      0      0.000000   -0.698997    4.323624
  26      1      0      0.000000   -1.206220    5.281576
-----------------------------------------------------------------
```
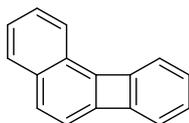

E = -615.4920952 a.u.

```
-----------------------------------------------------------------
Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number   Type          X        Y        Z
-----------------------------------------------------------------
```

1	6	0	3.103158	-2.678524	0.000000
2	6	0	1.761365	-3.061043	0.000000
3	6	0	0.739743	-2.113558	0.000000
4	6	0	1.099965	-0.727245	0.000000
5	6	0	2.450691	-0.358926	0.000000
6	6	0	3.445871	-1.329568	0.000000
7	1	0	-0.847829	-3.600714	0.000000
8	1	0	3.878481	-3.435060	0.000000
9	1	0	1.502820	-4.114837	0.000000
10	6	0	-0.660094	-2.532986	0.000000
11	6	0	0.000000	0.169637	0.000000
12	1	0	2.709838	0.693987	0.000000
13	1	0	4.488386	-1.034228	0.000000
14	6	0	-1.403485	-0.299743	0.000000
15	6	0	-1.725407	-1.650106	0.000000
16	1	0	-2.746090	-2.012610	0.000000
17	6	0	-1.839596	1.074251	0.000000
18	6	0	-0.455852	1.520401	0.000000
19	6	0	-2.900874	1.975158	0.000000
20	1	0	-3.938207	1.663521	0.000000
21	6	0	-0.128476	2.883284	0.000000
22	1	0	0.892286	3.244759	0.000000
23	6	0	-1.199139	3.759331	0.000000
24	1	0	-1.010608	4.826523	0.000000
25	6	0	-2.553517	3.319453	0.000000
26	1	0	-3.335195	4.069763	0.000000
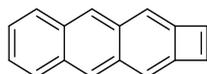
E = -615.4483894 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-0.684828	-4.305592
2	6	0	0.000000	-1.391772	-3.074410
3	6	0	0.000000	-0.718935	-1.859556
4	6	0	0.000000	0.718935	-1.859556
5	6	0	0.000000	1.391772	-3.074410
6	6	0	0.000000	0.684828	-4.305592
7	6	0	0.000000	-1.398905	-0.605776
8	6	0	0.000000	1.398905	-0.605776
9	6	0	0.000000	0.703963	0.659667
10	6	0	0.000000	-0.703963	0.659667
11	6	0	0.000000	-1.437180	1.883909
12	1	0	0.000000	-2.521076	1.862762
13	6	0	0.000000	-0.705818	3.033750
14	6	0	0.000000	0.705818	3.033750
15	6	0	0.000000	1.437180	1.883909
16	1	0	0.000000	-2.483213	-0.600847
17	1	0	0.000000	-1.236379	-5.237718
18	1	0	0.000000	-2.476248	-3.077970
19	1	0	0.000000	2.476248	-3.077970
20	1	0	0.000000	1.236379	-5.237718
21	1	0	0.000000	2.483213	-0.600847
22	1	0	0.000000	2.521076	1.862762
23	6	0	0.000000	0.672408	4.555139
24	1	0	0.000000	1.424652	5.330988
25	6	0	0.000000	-0.672408	4.555139
26	1	0	0.000000	-1.424652	5.330988
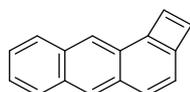
E = -615.4901595 a.u.

```
-----------------------------------------------------------------
Center     Atomic     Atomic            Coordinates (Angstroms)
Number     Number      Type         X          Y          Z
-----------------------------------------------------------------
   1         6         0        1.473505   -3.951039    0.000000
   2         6         0        0.247317   -3.338356    0.000000
   3         6         0        0.141552   -1.924866    0.000000
   4         6         0        1.334733   -1.143607    0.000000
   5         6         0        2.589308   -1.807876    0.000000
   6         6         0        2.658220   -3.175904    0.000000
   7         6         0       -1.113108   -1.269495    0.000000
   8         6         0        1.232417    0.263257    0.000000
   9         6         0        0.000000    0.894840    0.000000
  10         6         0       -1.220900    0.104761    0.000000
  11         6         0       -2.523111    0.746977    0.000000
  12         1         0       -3.389698    0.095368    0.000000
  13         6         0       -2.697229    2.119022    0.000000
  14         6         0       -1.538709    2.889842    0.000000
  15         6         0       -0.208411    2.294746    0.000000
  16         1         0       -2.014758   -1.875173    0.000000
  17         1         0        1.541091   -5.032257    0.000000
  18         1         0       -0.662794   -3.928778    0.000000
  19         1         0        3.494653   -1.210306    0.000000
  20         1         0        3.621395   -3.671886    0.000000
  21         1         0        2.139126    0.859780    0.000000
  22         1         0       -3.689594    2.553013    0.000000
  23         6         0       -0.928413    4.196590    0.000000
  24         1         0       -1.294561    5.212000    0.000000
  25         6         0        0.366528    3.601869    0.000000
  26         1         0        1.372947    3.993670    0.000000
-----------------------------------------------------------------
```
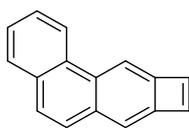

E = -615.485047 a.u.

```
-----------------------------------------------------------------
Center     Atomic     Atomic            Coordinates (Angstroms)
Number     Number      Type         X          Y          Z
-----------------------------------------------------------------
   1         6         0        2.942574   -2.813387    0.000000
   2         6         0        1.598453   -3.119504    0.000000
   3         6         0        0.623763   -2.106250    0.000000
   4         6         0        1.016795   -0.747023    0.000000
   5         6         0        2.396830   -0.463421    0.000000
   6         6         0        3.340256   -1.470727    0.000000
   7         6         0       -0.776287   -2.445728    0.000000
   8         6         0        0.000000    0.304570    0.000000
   9         6         0       -1.397186   -0.088127    0.000000
  10         6         0       -1.726911   -1.485964    0.000000
  11         6         0       -2.441834    0.854423    0.000000
  12         1         0       -3.471167    0.514347    0.000000
  13         6         0       -2.084417    2.187650    0.000000
  14         6         0       -0.677293    2.590375    0.000000
  15         6         0        0.352601    1.663017    0.000000
  16         1         0       -1.050148   -3.495233    0.000000
  17         1         0        3.684187   -3.602986    0.000000
  18         1         0        1.271443   -4.153958    0.000000
  19         1         0        2.743109    0.561124    0.000000
  20         1         0        4.393946   -1.218040    0.000000
  21         1         0       -2.777837   -1.754900    0.000000
  22         1         0        1.386081    1.980042    0.000000
  23         6         0       -2.483272    3.550457    0.000000
  24         1         0       -3.424002    4.078732    0.000000
  25         6         0       -1.054718    3.954971    0.000000
  26         1         0       -0.531736    4.898879    0.000000
-----------------------------------------------------------------
```
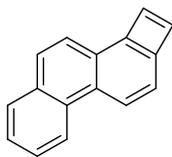
E = -615.4906829 a.u.

```
---------------------------------------------------------------------
Center    Atomic    Atomic        Coordinates (Angstroms)
Number    Number    Type        X         Y         Z
---------------------------------------------------------------------
   1        6        0       3.852098  -1.340176   0.000000
   2        6        0       2.711839  -2.104009   0.000000
   3        6        0       1.432237  -1.505274   0.000000
   4        6        0       1.315003  -0.088268   0.000000
   5        6        0       2.512223   0.669910   0.000000
   6        6        0       3.744943   0.063135   0.000000
   7        6        0       0.258047  -2.321037   0.000000
   8        6        0       0.000000   0.512773   0.000000
   9        6        0      -1.129845  -0.343665   0.000000
  10        6        0      -0.978042  -1.760664   0.000000
  11        6        0      -2.387269   0.296904   0.000000
  12        6        0      -2.526863   1.740967   0.000000
  13        6        0      -1.408280   2.572279   0.000000
  14        6        0      -0.175985   1.944157   0.000000
  15        1        0       0.378874  -3.398793   0.000000
  16        1        0       4.827907  -1.810436   0.000000
  17        1        0       2.775373  -3.186926   0.000000
  18        1        0       2.471992   1.750276   0.000000
  19        1        0       4.641637   0.671601   0.000000
  20        1        0      -1.869892  -2.377255   0.000000
  21        1        0      -1.476942   3.653074   0.000000
  22        1        0       0.704618   2.571046   0.000000
  23        6        0      -3.950664   1.601774   0.000000
  24        1        0      -4.791105   2.278315   0.000000
  25        6        0      -3.798785   0.149767   0.000000
  26        1        0      -4.486408  -0.682344   0.000000
---------------------------------------------------------------------
```
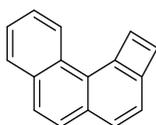

E = -615.4945008 a.u.

```
---------------------------------------------------------------------
Center    Atomic    Atomic        Coordinates (Angstroms)
Number    Number    Type        X         Y         Z
---------------------------------------------------------------------
   1        6        0       0.241753  -3.818511   0.000000
   2        6        0      -0.984068  -3.198605   0.000000
   3        6        0      -1.082584  -1.789339   0.000000
   4        6        0       0.101774  -1.010104   0.000000
   5        6        0       1.349085  -1.672181   0.000000
   6        6        0       1.419190  -3.045367   0.000000
   7        6        0      -2.351438  -1.134192   0.000000
   8        6        0       0.000000   0.425045   0.000000
   9        6        0      -1.275296   1.045907   0.000000
  10        6        0      -2.439127   0.225539   0.000000
  11        6        0      -1.423450   2.479792   0.000000
  12        1        0      -2.435604   2.869326   0.000000
  13        6        0      -0.355986   3.353341   0.000000
  14        6        0       0.909047   2.764815   0.000000
  15        6        0       1.093183   1.317791   0.000000
  16        1        0      -3.248999  -1.743116   0.000000
  17        1        0       0.306180  -4.899946   0.000000
```

18	1	0	-1.897097	-3.784503	0.000000
19	1	0	2.259633	-1.087532	0.000000
20	1	0	2.384640	-3.537128	0.000000
21	1	0	-3.410509	0.708319	0.000000
22	1	0	-0.506123	4.425697	0.000000
23	6	0	2.323926	2.948373	0.000000
24	1	0	2.988510	3.798288	0.000000
25	6	0	2.505084	1.505546	0.000000
26	1	0	3.372813	0.863501	0.000000
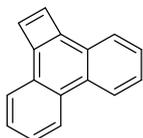
E = -615.4968295 a.u.

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |

1	6	0	0.000000	-3.579558	-0.750979
2	6	0	0.000000	-2.892258	0.443865
3	6	0	0.000000	-1.484357	0.461022
4	6	0	0.000000	-0.743095	-0.760728
5	6	0	0.000000	-1.479757	-1.952204
6	6	0	0.000000	-2.866452	-1.954347
7	6	0	0.000000	-0.720107	1.651042
8	6	0	0.000000	0.743095	-0.760728
9	6	0	0.000000	1.484357	0.461022
10	6	0	0.000000	0.720107	1.651042
11	6	0	0.000000	2.892258	0.443865
12	1	0	0.000000	3.423465	1.389001
13	6	0	0.000000	3.579558	-0.750979
14	6	0	0.000000	2.866452	-1.954347
15	6	0	0.000000	1.479757	-1.952204
16	1	0	0.000000	-4.662749	-0.759246
17	1	0	0.000000	-3.423465	1.389001
18	1	0	0.000000	-0.972920	-2.907467
19	1	0	0.000000	-3.397870	-2.898301
20	1	0	0.000000	4.662749	-0.759246
21	1	0	0.000000	3.397870	-2.898301
22	1	0	0.000000	0.972920	-2.907467
23	6	0	0.000000	-0.719528	3.082810
24	1	0	0.000000	-1.475695	3.853125
25	6	0	0.000000	0.719528	3.082810
26	1	0	0.000000	1.475695	3.853125
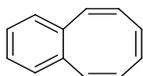
E = -463.0938797 a.u.

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |

1	6	0	0.000000	-0.702667	3.039072
2	6	0	0.000000	0.702667	3.039072
3	6	0	0.000000	1.366063	1.839636
4	6	0	0.000000	0.720967	0.566537
5	6	0	0.000000	-0.720967	0.566537
6	6	0	0.000000	-1.366063	1.839636
7	1	0	0.000000	-1.258197	3.968707
8	1	0	0.000000	1.258197	3.968707
9	1	0	0.000000	2.449780	1.848102
10	1	0	0.000000	-2.449780	1.848102

11	6	0	0.000000	1.654480	-0.513965
12	1	0	0.000000	2.672338	-0.137113
13	6	0	0.000000	-1.654480	-0.513965
14	1	0	0.000000	-2.672338	-0.137113
15	6	0	0.000000	1.657471	-1.919568
16	1	0	0.000000	2.671623	-2.309002
17	6	0	0.000000	-1.657471	-1.919568
18	1	0	0.000000	-2.671623	-2.309002
19	6	0	0.000000	0.710379	-2.920261
20	1	0	0.000000	1.135177	-3.919404
21	6	0	0.000000	-0.710379	-2.920261
22	1	0	0.000000	-1.135177	-3.919404
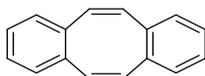
E = -616.7004681 a.u.

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |

1	6	0	0.000000	0.710394	4.253360
2	6	0	0.000000	-0.710394	4.253360
3	6	0	0.000000	-1.375746	3.065684
4	6	0	0.000000	-0.724345	1.784867
5	6	0	0.000000	0.724345	1.784867
6	6	0	0.000000	1.375746	3.065684
7	1	0	0.000000	1.259652	5.186706
8	1	0	0.000000	-1.259652	5.186706
9	1	0	0.000000	-2.459596	3.070593
10	1	0	0.000000	2.459596	3.070593
11	6	0	0.000000	-1.622982	0.700171
12	1	0	0.000000	-2.648143	1.059002
13	6	0	0.000000	1.622982	0.700171
14	1	0	0.000000	2.648143	1.059002
15	6	0	0.000000	-1.622982	-0.700171
16	1	0	0.000000	-2.648143	-1.059002
17	6	0	0.000000	1.622982	-0.700171
18	1	0	0.000000	2.648143	-1.059002
19	6	0	0.000000	-0.724345	-1.784867
20	6	0	0.000000	0.724345	-1.784867
21	6	0	0.000000	1.375746	-3.065684
22	1	0	0.000000	2.459596	-3.070593
23	6	0	0.000000	-1.375746	-3.065684
24	1	0	0.000000	-2.459596	-3.070593
25	6	0	0.000000	0.710394	-4.253360
26	1	0	0.000000	1.259652	-5.186706
27	6	0	0.000000	-0.710394	-4.253360
28	1	0	0.000000	-1.259652	-5.186706
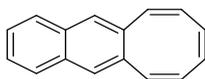
E = -616.7073781 a.u.

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |

1	6	0	0.000000	0.711873	4.266595
2	6	0	0.000000	1.404637	3.089364
3	6	0	0.000000	0.711547	1.845722
4	6	0	0.000000	-0.711547	1.845722
5	6	0	0.000000	-1.404637	3.089364
6	6	0	0.000000	-0.711873	4.266595
7	1	0	0.000000	2.453360	0.629388
8	1	0	0.000000	1.243355	5.210614

9	1	0	0.000000	2.489261	3.084281
10	6	0	0.000000	1.368548	0.612996
11	6	0	0.000000	-1.368548	0.612996
12	1	0	0.000000	-2.489261	3.084281
13	1	0	0.000000	-1.243355	5.210614
14	6	0	0.000000	-0.731004	-0.638440
15	6	0	0.000000	0.731004	-0.638440
16	1	0	0.000000	-2.453360	0.629388
17	6	0	0.000000	-1.658776	-1.725577
18	1	0	0.000000	-2.677957	-1.353081
19	6	0	0.000000	1.658776	-1.725577
20	1	0	0.000000	2.677957	-1.353081
21	6	0	0.000000	-1.657739	-3.137309
22	1	0	0.000000	-2.672424	-3.525533
23	6	0	0.000000	1.657739	-3.137309
24	1	0	0.000000	2.672424	-3.525533
25	6	0	0.000000	-0.715915	-4.132221
26	6	0	0.000000	0.715915	-4.132221
27	1	0	0.000000	1.137945	-5.132439
28	1	0	0.000000	-1.137945	-5.132439
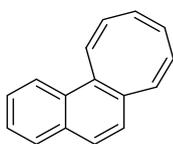
E = -616.7063033 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	3.225599	-2.590371	0.000000
2	6	0	1.911776	-2.989241	0.000000
3	6	0	0.863445	-2.048608	0.000000
4	6	0	1.119872	-0.652456	0.000000
5	6	0	2.490536	-0.285904	0.000000
6	6	0	3.506130	-1.217994	0.000000
7	1	0	-0.674160	-3.579450	0.000000
8	1	0	4.028260	-3.317398	0.000000
9	1	0	1.654367	-4.043019	0.000000
10	6	0	-0.485219	-2.511970	0.000000
11	6	0	0.000000	0.320512	0.000000
12	1	0	2.803052	0.746453	0.000000
13	1	0	4.534037	-0.875147	0.000000
14	6	0	-1.341897	-0.202406	0.000000
15	6	0	-1.508670	-1.630865	0.000000
16	1	0	-2.521657	-2.014156	0.000000
17	6	0	0.392416	1.679388	0.000000
18	1	0	1.463172	1.785395	0.000000
19	6	0	-0.157619	2.976606	0.000000
20	1	0	0.632923	3.722067	0.000000
21	6	0	-2.612566	0.451739	0.000000
22	1	0	-3.405592	-0.288823	0.000000
23	6	0	-3.179368	1.729559	0.000000
24	1	0	-4.264377	1.678262	0.000000
25	6	0	-2.710281	3.033762	0.000000
26	1	0	-3.494551	3.784308	0.000000
27	6	0	-1.410069	3.563695	0.000000
28	1	0	-1.379988	4.648831	0.000000
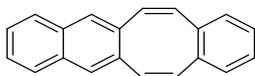
E = -770.310041 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.000000	0.715441	5.481273
2	6	0	0.000000	1.407548	4.309121
3	6	0	0.000000	0.715981	3.057557
4	6	0	0.000000	-0.715981	3.057557
5	6	0	0.000000	-1.407548	4.309121
6	6	0	0.000000	-0.715441	5.481273
7	1	0	0.000000	2.459508	1.848329
8	1	0	0.000000	1.244846	6.426455
9	1	0	0.000000	2.492121	4.304520
10	6	0	0.000000	1.374542	1.836306
11	6	0	0.000000	-1.374542	1.836306
12	1	0	0.000000	-2.492121	4.304520
13	1	0	0.000000	-1.244846	6.426455
14	6	0	0.000000	-0.728876	0.580577
15	6	0	0.000000	0.728876	0.580577
16	1	0	0.000000	-2.459508	1.848329
17	6	0	0.000000	-1.626897	-0.515287
18	1	0	0.000000	-2.652232	-0.157952
19	6	0	0.000000	1.626897	-0.515287
20	1	0	0.000000	2.652232	-0.157952
21	6	0	0.000000	-1.623371	-1.917944
22	1	0	0.000000	-2.649003	-2.275686
23	6	0	0.000000	1.623371	-1.917944
24	1	0	0.000000	2.649003	-2.275686
25	6	0	0.000000	-0.729874	-2.993463
26	6	0	0.000000	0.729874	-2.993463
27	6	0	0.000000	-1.380370	-4.283316
28	1	0	0.000000	-2.464208	-4.287967
29	6	0	0.000000	1.380370	-4.283316
30	1	0	0.000000	2.464208	-4.287967
31	6	0	0.000000	-0.715327	-5.464499
32	1	0	0.000000	-1.261466	-6.399645
33	6	0	0.000000	0.715327	-5.464499
34	1	0	0.000000	1.261466	-6.399645
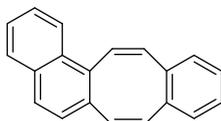
E = -770.318215 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.697392	5.184127	0.000000
2	6	0	0.581878	4.669017	0.000000
3	6	0	0.808664	3.284602	0.000000
4	6	0	-0.266007	2.361740	0.000000
5	6	0	-1.559533	2.927228	0.000000
6	6	0	-1.771833	4.294758	0.000000
7	1	0	2.972101	3.515309	0.000000
8	1	0	-0.864287	6.254161	0.000000
9	1	0	1.441489	5.330611	0.000000
10	6	0	2.159885	2.797256	0.000000
11	6	0	0.000000	0.894861	0.000000
12	1	0	-2.446874	2.312983	0.000000
13	1	0	-2.788306	4.669707	0.000000
14	6	0	1.390887	0.460020	0.000000
15	6	0	2.413451	1.473182	0.000000
16	1	0	3.443707	1.137957	0.000000
17	6	0	-1.125635	0.072563	0.000000
18	1	0	-2.036310	0.648043	0.000000
19	6	0	-1.507331	-1.283484	0.000000
20	1	0	-2.591935	-1.340138	0.000000
21	6	0	1.938622	-0.840145	0.000000
22	1	0	3.022443	-0.777136	0.000000

23	6	0	1.576083	-2.182765	0.000000
24	1	0	2.468241	-2.802405	0.000000
25	6	0	0.412414	-2.995928	0.000000
26	6	0	-0.963160	-2.588945	0.000000
27	6	0	0.685123	-4.396160	0.000000
28	6	0	-1.951671	-3.624678	0.000000
29	1	0	-2.992923	-3.322382	0.000000
30	6	0	-1.647168	-4.956733	0.000000
31	1	0	-2.437673	-5.697027	0.000000
32	6	0	-0.291862	-5.354004	0.000000
33	1	0	-0.026706	-6.404223	0.000000
34	1	0	1.724551	-4.704538	0.000000
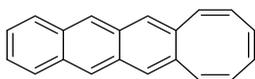
E = -770.2562409 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.688559	5.554316
2	6	0	0.000000	1.390399	4.332271
3	6	0	0.000000	0.716653	3.116978
4	6	0	0.000000	-0.716653	3.116978
5	6	0	0.000000	-1.390399	4.332271
6	6	0	0.000000	-0.688559	5.554316
7	6	0	0.000000	1.408911	1.861387
8	6	0	0.000000	-1.408911	1.861387
9	6	0	0.000000	-0.710195	0.615265
10	6	0	0.000000	0.710195	0.615265
11	6	0	0.000000	1.356263	-0.614133
12	1	0	0.000000	2.441063	-0.607067
13	6	0	0.000000	0.702211	-1.871074
14	6	0	0.000000	-0.702211	-1.871074
15	6	0	0.000000	-1.356263	-0.614133
16	1	0	0.000000	2.493063	1.859907
17	1	0	0.000000	1.237725	6.487816
18	1	0	0.000000	2.474994	4.333783
19	1	0	0.000000	-2.474994	4.333783
20	1	0	0.000000	-1.237725	6.487816
21	1	0	0.000000	-2.493063	1.859907
22	1	0	0.000000	-2.441063	-0.607067
23	6	0	0.000000	-1.671668	-2.990403
24	1	0	0.000000	-2.682911	-2.594429
25	6	0	0.000000	1.671668	-2.990403
26	1	0	0.000000	2.682911	-2.594429
27	6	0	0.000000	1.671644	-4.332930
28	1	0	0.000000	2.676753	-4.745554
29	6	0	0.000000	-1.671644	-4.332930
30	1	0	0.000000	-2.676753	-4.745554
31	6	0	0.000000	-0.668916	-5.396730
32	1	0	0.000000	-1.121060	-6.384151
33	6	0	0.000000	0.668916	-5.396730
34	1	0	0.000000	1.121060	-6.384151
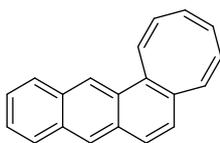
E = -770.3199002 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	2.928703	4.409806	0.000000
2	6	0	1.574825	4.225821	0.000000
3	6	0	1.025153	2.913871	0.000000
4	6	0	1.898616	1.792220	0.000000
5	6	0	3.304479	2.020631	0.000000
6	6	0	3.805130	3.291758	0.000000
7	6	0	-0.353056	2.660635	0.000000
8	6	0	1.366568	0.489474	0.000000
9	6	0	0.000000	0.219650	0.000000
10	6	0	-0.861342	1.373331	0.000000
11	6	0	-2.279777	1.177566	0.000000
12	1	0	-2.926544	2.047628	0.000000
13	6	0	-2.800272	-0.065391	0.000000
14	6	0	-2.016255	-1.276645	0.000000
15	6	0	-0.579618	-1.154172	0.000000
16	1	0	-1.046716	3.495864	0.000000
17	1	0	3.341746	5.411329	0.000000
18	1	0	0.900025	5.074928	0.000000
19	1	0	3.972005	1.165501	0.000000
20	1	0	4.876133	3.454440	0.000000
21	1	0	2.108120	-0.295476	0.000000
22	1	0	-3.877928	-0.174120	0.000000
23	6	0	0.368607	-2.198524	0.000000
24	1	0	1.376767	-1.821724	0.000000
25	6	0	0.448762	-3.602332	0.000000
26	1	0	1.487248	-3.922182	0.000000
27	6	0	-2.864121	-2.423259	0.000000
28	1	0	-3.903208	-2.110312	0.000000
29	6	0	-2.808359	-3.817601	0.000000
30	1	0	-3.804271	-4.251070	0.000000
31	6	0	-0.416952	-4.688304	0.000000
32	1	0	0.092906	-5.646658	0.000000
33	6	0	-1.809656	-4.785837	0.000000
34	1	0	-2.184889	-5.804341	0.000000
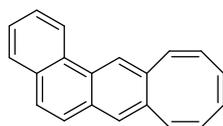
E = -770.3302999 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.660862	-2.373021	0.000000
2	6	0	-1.325077	-2.569190	0.000000
3	6	0	-0.419586	-1.453412	0.000000
4	6	0	-0.927827	-0.125022	0.000000
5	6	0	-2.372389	0.085842	0.000000
6	6	0	-3.223943	-1.044490	0.000000
7	1	0	1.314487	-2.667050	0.000000
8	1	0	-3.343422	-3.215855	0.000000
9	1	0	-0.910571	-3.571347	0.000000
10	6	0	0.956602	-1.642799	0.000000
11	6	0	0.000000	0.906753	0.000000
12	6	0	1.405164	0.747251	0.000000
13	6	0	1.916499	-0.612203	0.000000
14	1	0	-0.363841	1.925510	0.000000
15	6	0	2.095737	1.995667	0.000000
16	1	0	1.391611	2.821365	0.000000
17	6	0	3.256941	-1.107448	0.000000
18	1	0	3.259340	-2.192704	0.000000
19	6	0	3.417020	2.487699	0.000000
20	1	0	3.426693	3.574013	0.000000
21	6	0	4.576531	-0.617235	0.000000
22	1	0	5.295024	-1.432139	0.000000
23	6	0	4.681647	1.952822	0.000000
24	6	0	5.181223	0.616782	0.000000
25	1	0	6.265803	0.569645	0.000000

26	1	0	5.469880	2.699422	0.000000
27	6	0	-2.963142	1.363436	0.000000
28	1	0	-2.342124	2.249861	0.000000
29	6	0	-4.619409	-0.866257	0.000000
30	1	0	-5.255980	-1.744755	0.000000
31	6	0	-5.173480	0.395328	0.000000
32	1	0	-6.249445	0.520822	0.000000
33	6	0	-4.334242	1.517820	0.000000
34	1	0	-4.761901	2.513274	0.000000
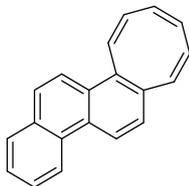
E = -770.3232619 a.u.

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |

1	6	0	-2.664976	1.624195	0.000000
2	6	0	-2.482360	0.223863	0.000000
3	6	0	-1.137250	-0.318520	0.000000
4	6	0	0.000000	0.517668	0.000000
5	6	0	-0.256312	1.934525	0.000000
6	6	0	-1.509411	2.454277	0.000000
7	1	0	-1.781563	-2.400163	0.000000
8	6	0	-0.939196	-1.724515	0.000000
9	6	0	1.367133	-0.040857	0.000000
10	1	0	0.545946	2.653259	0.000000
11	1	0	-1.644215	3.530610	0.000000
12	6	0	1.508994	-1.473646	0.000000
13	6	0	0.310238	-2.250650	0.000000
14	1	0	0.410750	-3.329139	0.000000
15	6	0	2.414244	0.914496	0.000000
16	1	0	2.040272	1.921771	0.000000
17	6	0	3.822971	0.997037	0.000000
18	1	0	4.137184	2.037379	0.000000
19	6	0	2.662564	-2.320207	0.000000
20	1	0	2.350745	-3.359457	0.000000
21	6	0	4.061096	-2.260891	0.000000
22	1	0	4.496478	-3.256089	0.000000
23	6	0	5.016986	-1.262504	0.000000
24	1	0	6.039636	-1.626170	0.000000
25	6	0	4.906631	0.142056	0.000000
26	1	0	5.863330	0.655259	0.000000
27	6	0	-3.643689	-0.587691	0.000000
28	1	0	-3.563026	-1.665364	0.000000
29	6	0	-3.964218	2.177065	0.000000
30	1	0	-4.069968	3.256625	0.000000
31	6	0	-5.070088	1.364821	0.000000
32	1	0	-6.066071	1.790718	0.000000
33	6	0	-4.901408	-0.032304	0.000000
34	1	0	-5.771199	-0.678543	0.000000
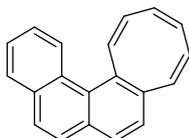
E = -770.3228822 a.u.

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |

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   2      6      0       2.237308    2.379216    0.237755
   3      6      0       0.873413    1.977347    0.127422
   4      6      0       0.525197    0.616778    0.086202
   5      6      0       1.596731   -0.350305   -0.074726
   6      6      0       2.945335    0.077402    0.064184
   7      1      0       0.114518    4.009056    0.101649
   8      1      0       4.270415    1.765300    0.374688
   9      1      0       2.454234    3.438571    0.320839
  10      6      0      -0.155674    2.959765    0.063921
  11      6      0      -0.873464    0.225924    0.211617
  12      6      0      -1.871511    1.214178   -0.116673
  13      6      0      -1.446575    2.582539   -0.122917
  14      1      0      -2.206323    3.341786   -0.270027
  15      6      0      -1.097320   -1.004494    0.885485
  16      1      0      -0.203185   -1.333710    1.404147
  17      6      0      -2.150181   -1.906379    1.088755
  18      1      0      -1.875132   -2.693650    1.785185
  19      6      0      -3.231418    1.049090   -0.480716
  20      1      0      -3.685410    2.002725   -0.735431
  21      6      0      -4.108968   -0.013134   -0.746135
  22      1      0      -4.982352    0.313031   -1.304782
  23      6      0      -4.167835   -1.347784   -0.385059
  24      1      0      -5.043773   -1.867427   -0.761599
  25      6      0      -3.390673   -2.114555    0.505991
  26      1      0      -3.853489   -3.056032    0.786969
  27      6      0       1.380506   -1.694157   -0.475088
  28      1      0       0.376977   -2.026545   -0.704241
  29      6      0       3.998651   -0.856470   -0.062485
  30      1      0       5.016411   -0.507003    0.074418
  31      6      0       3.748430   -2.166468   -0.384637
  32      1      0       4.563773   -2.871999   -0.489791
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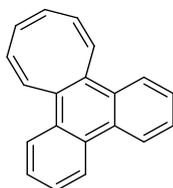

E = -770.3120485 a.u.

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Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number    Type       X         Y         Z
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   3      6      0       0.000000    1.439012   -0.510370
   4      6      0       0.000000    0.731627   -1.733404
   5      6      0       0.000000    1.438234   -2.951851
   6      6      0       0.000000    2.812436   -3.006457
   7      6      0       0.000000    0.718335    0.791929
   8      6      0       0.000000   -0.731627   -1.733404
   9      6      0       0.000000   -1.439012   -0.510370
  10      6      0       0.000000   -0.718335    0.791929
  11      6      0       0.000000   -2.855570   -0.608380
  12      1      0       0.000000   -3.489035    0.262460
  13      6      0       0.000000   -3.526840   -1.810366
  14      6      0       0.000000   -2.812436   -3.006457
  15      6      0       0.000000   -1.438234   -2.951851
  16      1      0       0.000000    4.610064   -1.813932
  17      1      0       0.000000    3.489035    0.262460
  18      1      0       0.000000    0.903988   -3.888630
  19      1      0       0.000000    3.323161   -3.961475
  20      1      0       0.000000   -4.610064   -1.813932
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21	1	0	0.000000	-3.323161	-3.961475
22	1	0	0.000000	-0.903988	-3.888630
23	6	0	0.000000	-1.578675	1.920524
24	1	0	0.000000	-2.606099	1.613143
25	6	0	0.000000	1.578675	1.920524
26	1	0	0.000000	2.606099	1.613143
27	6	0	0.000000	1.603072	3.324972
28	1	0	0.000000	2.628871	3.683307
29	6	0	0.000000	-1.603072	3.324972
30	1	0	0.000000	-2.628871	3.683307
31	6	0	0.000000	-0.697256	4.374510
32	1	0	0.000000	-1.155219	5.358490
33	6	0	0.000000	0.697256	4.374510
34	1	0	0.000000	1.155219	5.358490
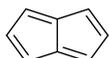
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	0.000000	-0.741131	0.000000
3	6	0	0.000000	0.741131	0.000000
4	6	0	0.000000	1.168704	-1.335065
5	1	0	0.000000	0.000000	-3.219661
6	1	0	0.000000	-2.183438	-1.703309
7	1	0	0.000000	2.183438	-1.703309
8	6	0	0.000000	0.000000	-2.137422
9	6	0	0.000000	1.168704	1.335065
10	1	0	0.000000	2.183438	1.703309
11	6	0	0.000000	-1.168704	1.335065
12	1	0	0.000000	-2.183438	1.703309
13	6	0	0.000000	0.000000	2.137422
14	1	0	0.000000	0.000000	3.219661
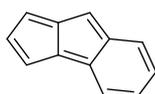
E = -461.9136612 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.666656	0.000000
2	6	0	1.071089	-0.274010	0.000000
3	6	0	0.494718	-1.619323	0.000000
4	6	0	-0.904149	-1.510775	0.000000
5	1	0	-1.629832	-2.310601	0.000000
6	6	0	-1.218851	-0.100133	0.000000
7	6	0	1.554157	-2.521226	0.000000
8	1	0	1.507529	-3.600040	0.000000
9	6	0	2.495790	-0.388641	0.000000
10	1	0	3.213314	0.417584	0.000000
11	6	0	2.782848	-1.736317	0.000000
12	1	0	3.776304	-2.164005	0.000000
13	6	0	-2.445522	0.562052	0.000000
14	1	0	-3.374234	0.003129	0.000000
15	6	0	-0.038440	2.062458	0.000000
16	1	0	0.880652	2.637327	0.000000
17	6	0	-2.460187	1.953340	0.000000
18	1	0	-3.410237	2.474914	0.000000
19	6	0	-1.271859	2.699341	0.000000

| 20 | 1 | 0 | -1.321059 | 3.781159 | 0.000000 |
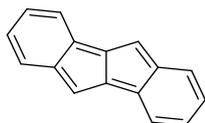
E = -615.5278641 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-0.807002	2.002522	0.000000
3	6	0	0.612121	1.661205	0.000000
4	6	0	1.589050	2.679890	0.000000
5	6	0	1.183557	3.990072	0.000000
6	6	0	-0.203334	4.325937	0.000000
7	1	0	-2.231546	3.640595	0.000000
8	1	0	2.642209	2.422896	0.000000
9	1	0	1.916442	4.787505	0.000000
10	1	0	-0.483639	5.373300	0.000000
11	6	0	0.692159	0.257688	0.000000
12	6	0	-1.590739	0.820654	0.000000
13	1	0	-2.669861	0.783364	0.000000
14	6	0	-0.692159	-0.257688	0.000000
15	6	0	-0.612121	-1.661205	0.000000
16	6	0	1.590739	-0.820654	0.000000
17	1	0	2.669861	-0.783364	0.000000
18	6	0	0.807002	-2.002522	0.000000
19	6	0	-1.589050	-2.679890	0.000000
20	1	0	-2.642209	-2.422896	0.000000
21	6	0	1.183557	-3.363518	0.000000
22	1	0	2.231546	-3.640595	0.000000
23	6	0	0.203334	-4.325937	0.000000
24	1	0	0.483639	-5.373300	0.000000
25	6	0	-1.183557	-3.990072	0.000000
26	1	0	-1.916442	-4.787505	0.000000
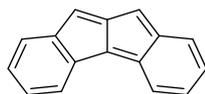
E = -615.5484546 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-3.564104	0.717733
2	6	0	0.000000	-2.181070	0.837033
3	6	0	0.000000	-1.363364	-0.340866
4	6	0	0.000000	-1.944865	-1.603010
5	6	0	0.000000	-3.336944	-1.703631
6	6	0	0.000000	-4.133181	-0.558526
7	1	0	0.000000	-4.194871	1.599583
8	1	0	0.000000	-1.331589	-2.496564
9	1	0	0.000000	-3.804710	-2.680506
10	1	0	0.000000	-5.211900	-0.661266
11	6	0	0.000000	0.000000	0.113752
12	6	0	0.000000	-1.327541	2.013470
13	1	0	0.000000	-1.678333	3.035176
14	6	0	0.000000	0.000000	1.563035
15	6	0	0.000000	1.327541	2.013470
16	6	0	0.000000	1.363364	-0.340866
17	6	0	0.000000	2.181070	0.837033

S107

18	6	0	0.000000	3.564104	0.717733
19	1	0	0.000000	4.194871	1.599583
20	6	0	0.000000	1.944865	-1.603010
21	1	0	0.000000	1.331589	-2.496564
22	6	0	0.000000	4.133181	-0.558526
23	1	0	0.000000	5.211900	-0.661266
24	6	0	0.000000	3.336944	-1.703631
25	1	0	0.000000	3.804710	-2.680506
26	1	0	0.000000	1.678333	3.035176
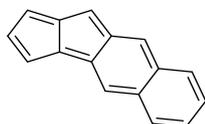
E = -615.5317489 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.785295	0.000000
2	6	0	1.244321	0.197983	0.000000
3	6	0	1.354728	-1.215592	0.000000
4	6	0	0.170275	-2.016300	0.000000
5	6	0	-1.111266	-1.398058	0.000000
6	6	0	-1.213368	-0.029983	0.000000
7	1	0	3.512159	-1.240648	0.000000
8	1	0	2.146462	0.801509	0.000000
9	6	0	2.618777	-1.856425	0.000000
10	6	0	0.308411	-3.425622	0.000000
11	1	0	-1.997171	-2.024914	0.000000
12	6	0	1.547213	-4.016366	0.000000
13	6	0	2.717759	-3.223966	0.000000
14	1	0	-0.589091	-4.035027	0.000000
15	1	0	1.631980	-5.096596	0.000000
16	1	0	3.690260	-3.700856	0.000000
17	6	0	-2.362637	0.844153	0.000000
18	1	0	-3.392178	0.518308	0.000000
19	6	0	-0.428421	2.143627	0.000000
20	6	0	-1.878110	2.164686	0.000000
21	6	0	0.054387	3.504096	0.000000
22	1	0	1.085282	3.824779	0.000000
23	6	0	-2.268962	3.505160	0.000000
24	1	0	-3.274248	3.900335	0.000000
25	6	0	-1.049139	4.313711	0.000000
26	1	0	-1.037266	5.394724	0.000000
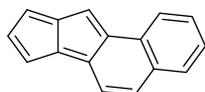
E = -615.5342995 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	2.051867	1.431664	0.000000
4	6	0	0.674282	1.699226	0.000000
5	1	0	0.200673	2.669411	0.000000
6	6	0	0.000000	0.434858	0.000000
7	6	0	3.313942	2.015772	0.000000
8	1	0	3.559063	3.067275	0.000000
9	6	0	3.623760	-0.300525	0.000000
10	1	0	4.105942	-1.266168	0.000000

11	6	0	4.269815	0.937708	0.000000
12	1	0	5.343043	1.075536	0.000000
13	6	0	-1.396056	0.134813	0.000000
14	6	0	0.541599	-1.984030	0.000000
15	1	0	1.281132	-2.776381	0.000000
16	6	0	-1.784279	-1.234740	0.000000
17	6	0	-0.792233	-2.272581	0.000000
18	1	0	-1.133014	-3.301900	0.000000
19	6	0	-3.159759	-1.547669	0.000000
20	1	0	-3.457650	-2.590861	0.000000
21	6	0	-2.393453	1.134729	0.000000
22	1	0	-2.096359	2.177162	0.000000
23	6	0	-3.726738	0.799046	0.000000
24	1	0	-4.482284	1.575383	0.000000
25	6	0	-4.112948	-0.554948	0.000000
26	1	0	-5.165186	-0.813818	0.000000
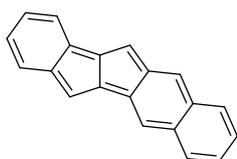
E = -769.1464317 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

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2	6	0	0.143003	1.989995	0.000000
3	6	0	-1.011284	2.817803	0.000000
4	6	0	-2.306830	2.216257	0.000000
5	6	0	-2.438541	0.793849	0.000000
6	6	0	-1.324153	0.001123	0.000000
7	1	0	0.081151	4.676434	0.000000
8	1	0	1.126352	2.449789	0.000000
9	6	0	-0.907257	4.228899	0.000000
10	6	0	-3.440565	3.058589	0.000000
11	1	0	-3.434626	0.362765	0.000000
12	6	0	-3.308614	4.427913	0.000000
13	6	0	-2.029360	5.021305	0.000000
14	1	0	-4.426065	2.605164	0.000000
15	1	0	-4.191620	5.056059	0.000000
16	1	0	-1.935096	6.100334	0.000000
17	6	0	-1.155610	-1.437806	0.000000
18	1	0	-1.960682	-2.157484	0.000000
19	6	0	0.931744	-0.451700	0.000000
20	6	0	0.215513	-1.683423	0.000000
21	6	0	2.371758	-0.723695	0.000000
22	1	0	3.169733	0.004065	0.000000
23	6	0	1.199189	-2.740581	0.000000
24	6	0	2.511269	-2.107276	0.000000
25	6	0	1.097704	-4.127236	0.000000
26	1	0	0.126492	-4.608168	0.000000
27	6	0	3.679412	-2.920947	0.000000
28	1	0	4.659948	-2.458538	0.000000
29	6	0	2.258844	-4.888817	0.000000
30	1	0	2.187935	-5.970036	0.000000
31	6	0	3.542858	-4.284925	0.000000
32	1	0	4.421999	-4.917799	0.000000
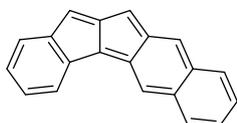
E = -769.1684921 a.u.

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Number     Number      Type        X          Y          Z
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   2         6          0      1.364144    0.455998    0.000000
   3         6          0      1.941854    1.757669    0.000000
   4         6          0      1.095322    2.906243    0.000000
   5         6          0     -0.321676    2.746258    0.000000
   6         6          0     -0.868722    1.490259    0.000000
   7         1          0      3.982124    1.062062    0.000000
   8         1          0      2.018123   -0.409529    0.000000
   9         6          0      3.344227    1.939715    0.000000
  10         6          0      1.691853    4.188258    0.000000
  11         1          0     -0.950483    3.630894    0.000000
  12         6          0      3.058232    4.334168    0.000000
  13         6          0      3.894536    3.198308    0.000000
  14         1          0      1.048130    5.061534    0.000000
  15         1          0      3.496987    5.324778    0.000000
  16         1          0      4.970619    3.322467    0.000000
  17         6          0     -2.245365    1.049726    0.000000
  18         1          0     -3.107433    1.700421    0.000000
  19         6          0     -0.866787   -0.821660    0.000000
  20         6          0     -2.234427   -0.356204    0.000000
  21         6          0     -0.873174   -2.263478    0.000000
  22         6          0     -3.088162   -1.469322    0.000000
  23         6          0     -2.250112   -2.658187    0.000000
  24         1          0     -4.168438   -1.471247    0.000000
  25         6          0      0.131664   -3.219703    0.000000
  26         1          0      1.175768   -2.929204    0.000000
  27         6          0     -2.585334   -4.004080    0.000000
  28         1          0     -3.623804   -4.315898    0.000000
  29         6          0     -1.561309   -4.957308    0.000000
  30         1          0     -1.813038   -6.011239    0.000000
  31         6          0     -0.223481   -4.572594    0.000000
  32         1          0      0.551743   -5.329202    0.000000
-----------------------------------------------------------------
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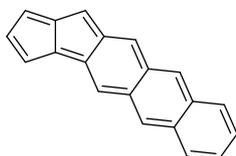

E = -769.1435914 a.u.

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-----------------------------------------------------------------
Center     Atomic      Atomic            Coordinates (Angstroms)
Number     Number      Type        X          Y          Z
-----------------------------------------------------------------
   1         6          0      1.618975   -1.061489    0.000000
   2         6          0      1.352285    0.284606    0.000000
   3         6          0      0.000000    0.741867    0.000000
   4         6          0     -1.074656   -0.223650    0.000000
   5         6          0     -0.773331   -1.625213    0.000000
   6         6          0      0.524373   -2.050018    0.000000
   7         1          0      0.507680    2.823992    0.000000
   8         1          0      2.155962    1.013956    0.000000
   9         6          0     -0.303571    2.101848    0.000000
  10         6          0     -2.386241    0.237735    0.000000
  11         1          0     -1.595393   -2.333446    0.000000
  12         6          0     -2.690680    1.605592    0.000000
  13         6          0     -1.624804    2.561396    0.000000
  14         1          0     -3.199813   -0.481416    0.000000
  15         6          0      1.099383   -3.370159    0.000000
  16         1          0      0.539144   -4.293175    0.000000
  17         6          0      2.827656   -1.805319    0.000000
  18         6          0      2.499155   -3.211931    0.000000
  19         6          0      4.270517   -1.666566    0.000000
```

S110

20	1	0	4.830201	-0.743323	0.000000
21	6	0	3.707550	-3.916376	0.000000
22	6	0	4.789258	-2.930479	0.000000
23	1	0	3.846116	-4.987780	0.000000
24	1	0	5.840663	-3.182033	0.000000
25	6	0	-4.035310	2.081242	0.000000
26	1	0	-4.842038	1.356221	0.000000
27	6	0	-1.944917	3.952183	0.000000
28	1	0	-1.132237	4.670709	0.000000
29	6	0	-3.243085	4.369316	0.000000
30	1	0	-3.475736	5.427467	0.000000
31	6	0	-4.303449	3.418902	0.000000
32	1	0	-5.329204	3.767902	0.000000
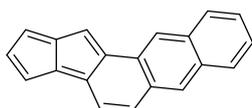
E = -769.1479908 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z

1	6	0	0.681319	-2.145443	0.000000
2	6	0	-0.353537	-1.141710	0.000000
3	6	0	0.000000	0.250015	0.000000
4	6	0	1.401461	0.588151	0.000000
5	6	0	2.397149	-0.460630	0.000000
6	6	0	2.053279	-1.776177	0.000000
7	1	0	-2.002390	1.014160	0.000000
8	6	0	-0.946474	1.264070	0.000000
9	6	0	1.768396	1.922092	0.000000
10	1	0	3.440227	-0.164353	0.000000
11	6	0	0.812954	2.955457	0.000000
12	6	0	-0.574437	2.618488	0.000000
13	1	0	2.814879	-2.547417	0.000000
14	6	0	-1.635059	-1.761869	0.000000
15	1	0	-2.586506	-1.251208	0.000000
16	6	0	0.032993	-3.396810	0.000000
17	6	0	-1.423042	-3.146435	0.000000
18	6	0	-2.067300	-4.387740	0.000000
19	1	0	-3.129330	-4.580915	0.000000
20	6	0	0.234895	-4.783078	0.000000
21	1	0	1.174267	-5.315039	0.000000
22	6	0	-1.045824	-5.377046	0.000000
23	1	0	-1.227204	-6.443919	0.000000
24	1	0	2.822552	2.183337	0.000000
25	6	0	1.184497	4.328707	0.000000
26	1	0	2.239271	4.582173	0.000000
27	6	0	-1.538721	3.665867	0.000000
28	1	0	-2.591344	3.403460	0.000000
29	6	0	-1.147621	4.974548	0.000000
30	1	0	-1.888183	5.765221	0.000000
31	6	0	0.232750	5.309862	0.000000
32	1	0	0.527691	6.352598	0.000000
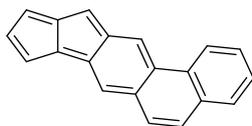
E = -769.1519076 a.u.

Center Number	Atomic Number	Atomic Type	X	Y	Z

1	6	0	0.199560	-1.879584	0.000000
2	6	0	1.352434	-1.121231	0.000000
3	6	0	1.269938	0.285301	0.000000
4	6	0	0.000000	0.932624	0.000000
5	6	0	-1.175023	0.147144	0.000000
6	6	0	-1.097142	-1.229715	0.000000
7	1	0	3.421489	0.546635	0.000000
8	1	0	2.329504	-1.593510	0.000000
9	6	0	2.471242	1.069649	0.000000
10	6	0	-0.040735	2.387711	0.000000
11	1	0	-2.150004	0.616297	0.000000
12	6	0	1.173483	3.117538	0.000000
13	6	0	2.428865	2.420993	0.000000
14	6	0	-2.132267	-2.235861	0.000000
15	1	0	-3.193802	-2.037677	0.000000
16	6	0	-0.049411	-3.282713	0.000000
17	6	0	-1.490983	-3.486618	0.000000
18	6	0	0.597199	-4.566450	0.000000
19	1	0	1.659538	-4.757243	0.000000
20	6	0	-1.711142	-4.862227	0.000000
21	6	0	-0.399864	-5.509148	0.000000
22	1	0	-2.658022	-5.381796	0.000000
23	1	0	-0.251856	-6.580281	0.000000
24	6	0	1.142738	4.527134	0.000000
25	6	0	-1.250228	3.116153	0.000000
26	1	0	-2.197746	2.594934	0.000000
27	6	0	-1.258174	4.493112	0.000000
28	1	0	-2.201815	5.025215	0.000000
29	6	0	-0.050792	5.209965	0.000000
30	1	0	-0.061777	6.293122	0.000000
31	1	0	3.342347	3.005348	0.000000
32	1	0	2.083954	5.066296	0.000000
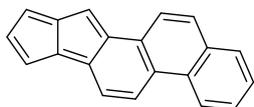
E = -769.1528682 a.u.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	1.558553	-1.241597	0.000000
2	6	0	1.325953	0.170937	0.000000
3	6	0	0.000000	0.672524	0.000000
4	6	0	-1.078166	-0.247043	0.000000
5	6	0	-0.805196	-1.646530	0.000000
6	6	0	0.476325	-2.137603	0.000000
7	1	0	0.583726	2.763896	0.000000
8	6	0	-0.257326	2.081439	0.000000
9	6	0	-2.435804	0.267635	0.000000
10	1	0	-1.625039	-2.350466	0.000000
11	6	0	-2.645994	1.669612	0.000000
12	6	0	-1.523340	2.559452	0.000000
13	6	0	-3.960405	2.183194	0.000000
14	6	0	-3.575121	-0.570329	0.000000
15	1	0	-3.459857	-1.645407	0.000000
16	6	0	-4.847770	-0.047921	0.000000
17	1	0	-5.701657	-0.714803	0.000000
18	6	0	-5.047541	1.343441	0.000000
19	1	0	-6.052703	1.747249	0.000000
20	1	0	-1.712097	3.627335	0.000000
21	1	0	-4.096415	3.259319	0.000000
22	1	0	0.653628	-3.206798	0.000000
23	6	0	2.583874	0.870715	0.000000
24	1	0	2.715293	1.942080	0.000000
25	6	0	2.965886	-1.429645	0.000000
26	6	0	3.595972	-0.100917	0.000000

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27      6       0     4.972206  -0.294191   0.000000
28      1       0     5.748952   0.455857   0.000000
29      6       0     3.987756  -2.411591   0.000000
30      1       0     3.865512  -3.483983   0.000000
31      6       0     5.194778  -1.725893   0.000000
32      1       0     6.172821  -2.188416   0.000000
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