

Electronic Supplementary Information

NICS Values for Neutral and Doubly Charged Polyacenes

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We first present tables of NICS values for neutral and doubly charged polyacenes in closed-shell electronic configuration. These NICS values were calculated at the B3LYP/6-31G* level of theory⁴² using the GIAO method.⁴⁹ They are presumably useful for many studies, although most of them were not referred to in the present study. In Tables S1–S3, species **1**, **2**, **3**, **4**, **5**, **6**, **7**, **8** and **9** represent benzene, naphthalene, anthracene, naphthacene, pentacene, hexacene, heptacene, octacene and nonacene, respectively. For types of rings in Tables S1-S3 and references cited in this Electronic Supplementary Information, see the text.

Fig. S1 shows a plot of the HOMA index against the peripheral BRE for all non-identical benzene rings in **1-9**. A good correlation with a correlation coefficient of 0.974 is found between these two quantities. Somewhat scattered points are due to benzene rings with BREs $< 0.150 |\beta|$, which implies that the HOMA index might be sensitive to the molecular geometry employed when the ring concerned is not highly aromatic.³⁴

Table S1 NICS values for neutral polyacene molecules in closed-shell electronic configuration.

Species	Ring a	Ring b	Ring c	Ring d	Ring e	Weighted average
1	-9.67					-9.67
2	-9.99					-9.99
3	-8.84	-12.60				-10.09
4	-7.83	-12.59				-10.21
5	-7.06	-12.05	-13.49			-10.34
6	-6.48	-11.42	-13.50			-10.47
7	-6.05	-10.85	-13.18	-13.94		-10.59
8	-5.74	-10.38	-12.78	-13.92		-10.71
9	-5.50	-9.99	-12.38	-13.71	-14.14	-10.81

Table S2 NICS values for the molecular dications of polyacenes in closed-shell electronic configuration.

Species	Ring a	Ring b	Ring c	Ring d	Ring e	Weighted average
1²⁺	88.34					88.34
2²⁺	30.83					30.83
3²⁺	10.94	16.37				12.75
4²⁺	2.89	8.21				5.55
5²⁺	-1.19	2.82	4.70			1.59
6²⁺	-3.44	-0.83	1.52			-0.92
7²⁺	-4.75	-3.37	-1.05	-0.24		-2.65
8²⁺	-5.54	-5.17	-3.09	-1.94		-3.93
9²⁺	-6.04	-6.48	-4.71	-3.43	-2.99	-4.92

Table S3 NICS values for the molecular dianions of polyacenes in closed-shell electronic configuration.

Species	Ring a	Ring b	Ring c	Ring d	Ring e	Weighted average
1²⁻	117.68					117.68
2²⁻	43.46					43.46
3²⁻	15.33	19.03				16.56
4²⁻	5.32	8.83				7.08
5²⁻	0.73	3.06	3.85			2.29
6²⁻	-1.57	-0.40	0.26			-0.57
7²⁻	-2.77	-2.52	-2.20	-2.27		-2.46
8²⁻	-3.37	-3.81	-3.85	-4.21		-3.81
9²⁻	-3.65	-4.55	-4.90	-5.60	-5.94	-4.82

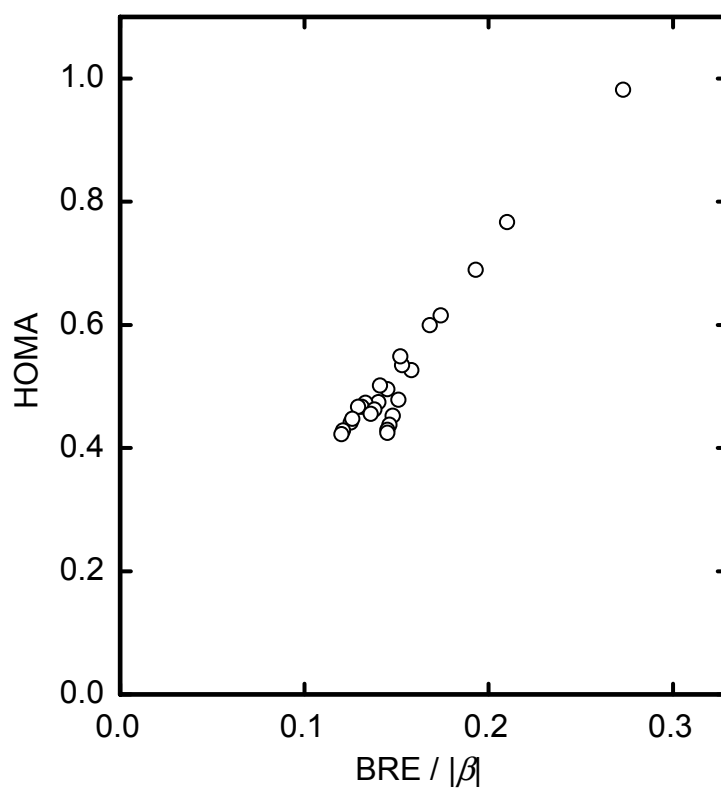


Fig. S1 Correlation between the local HOMA index and the peripheral BRE for all non-identical benzene rings in **1-9**.