Supporting Information

Aromatic Character of Nanographene Model Compounds

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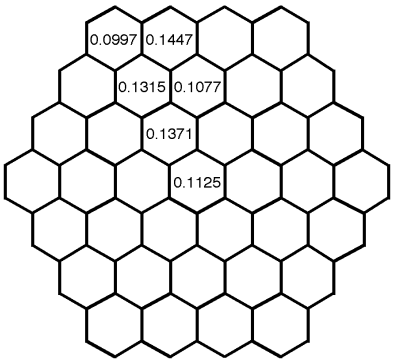
■ SSEs for Benzene Rings in Nanographene Model Compounds Studied

Superaromatic stabilization energies (SSEs)[S1,S2] for all nonidentical benzene rings of nanographene model compounds **1-40** are graphically summarized below:



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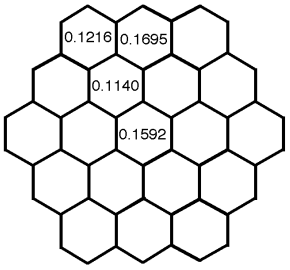

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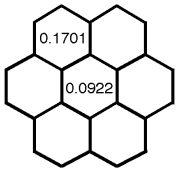

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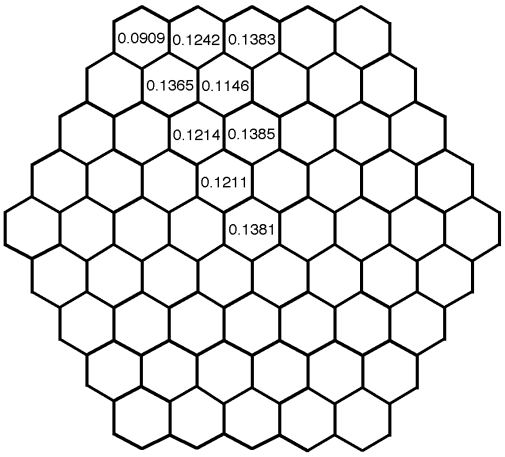

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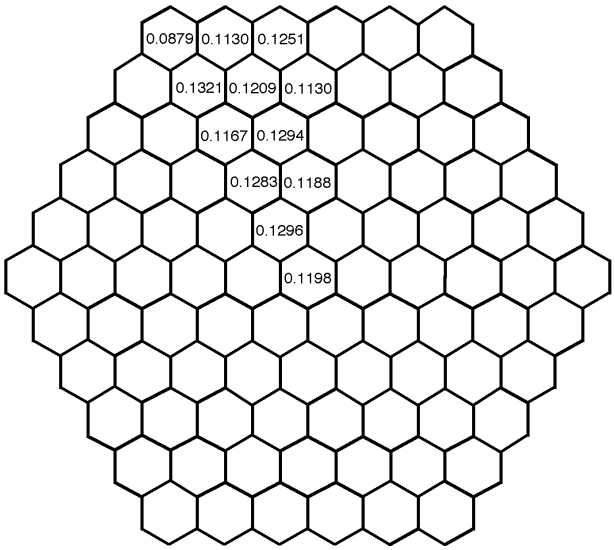

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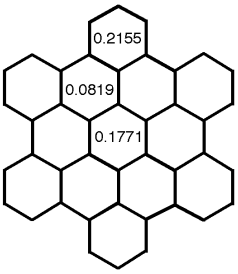
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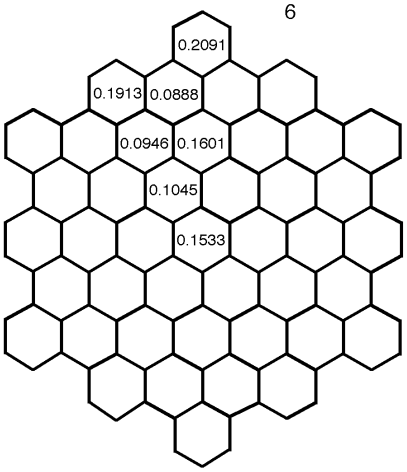
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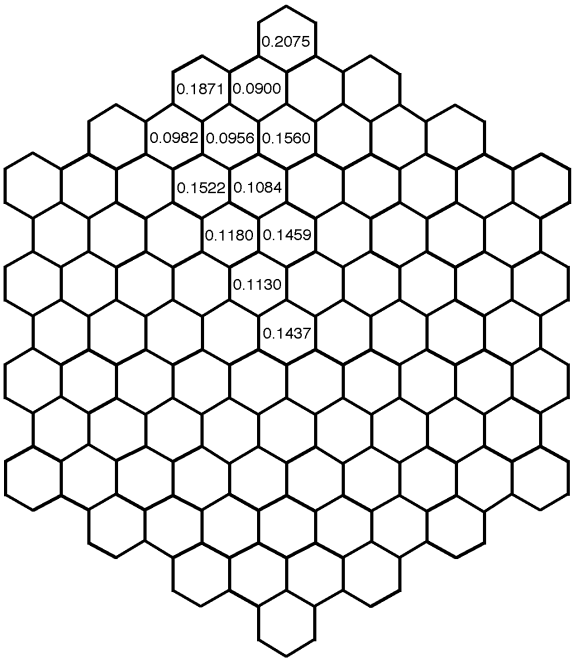
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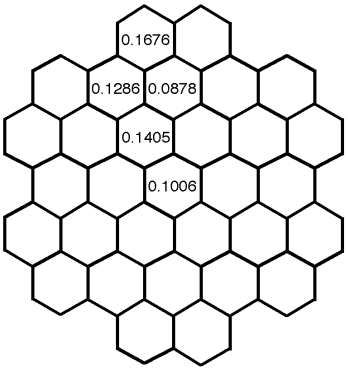
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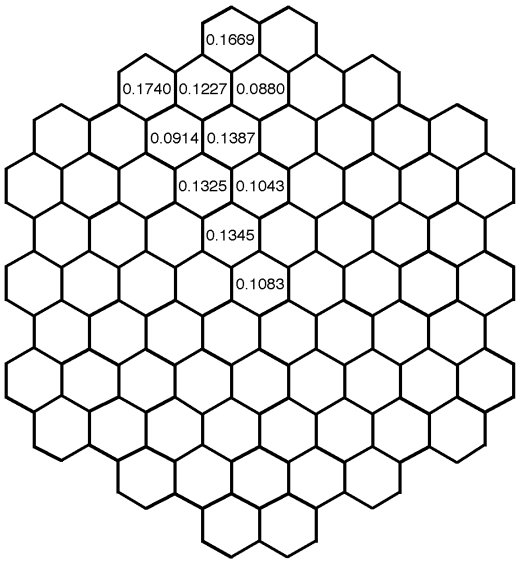
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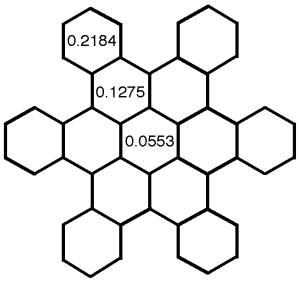
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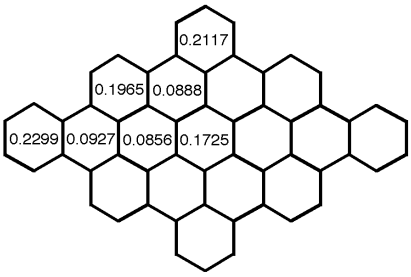
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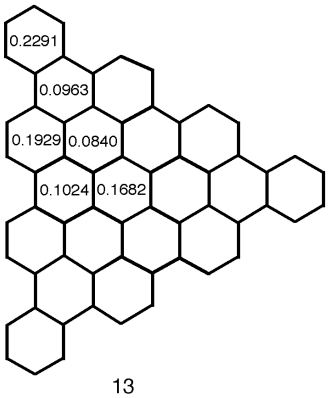
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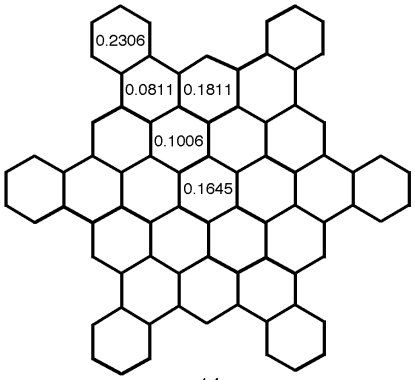
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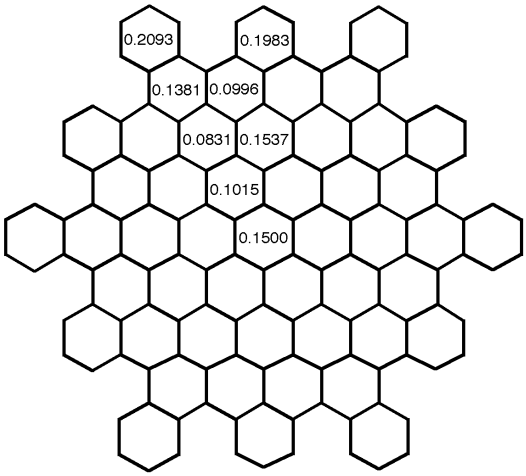
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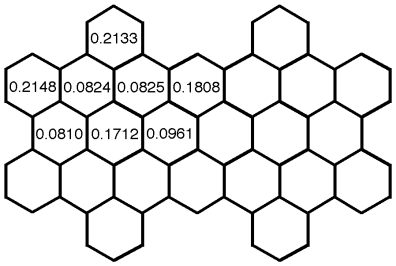

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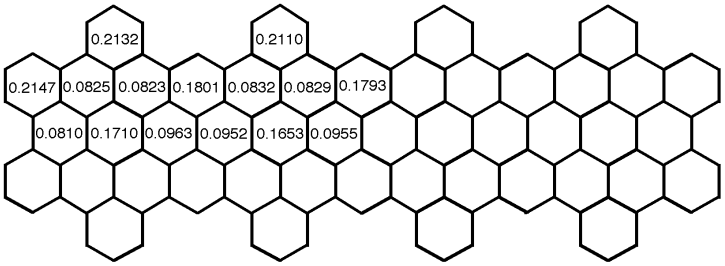

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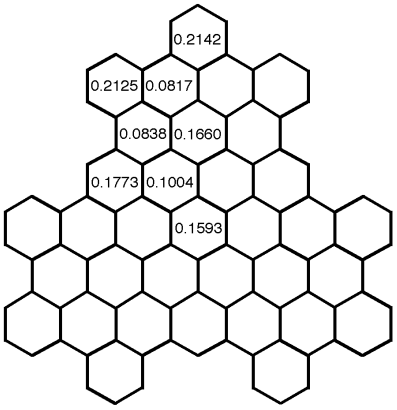

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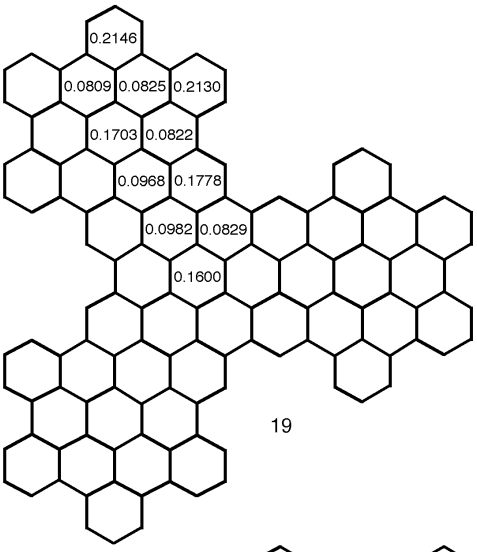

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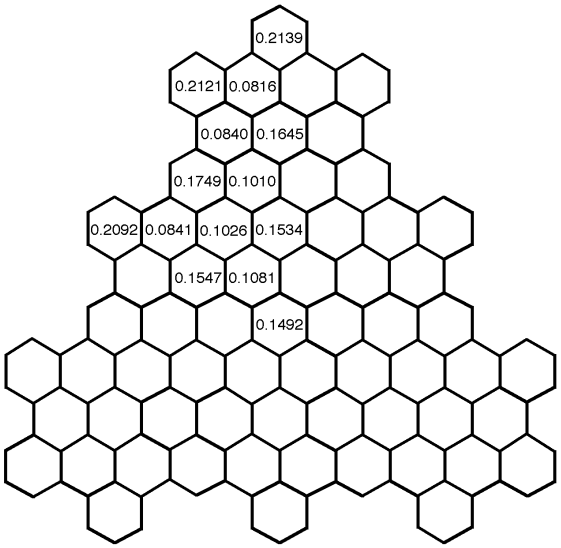

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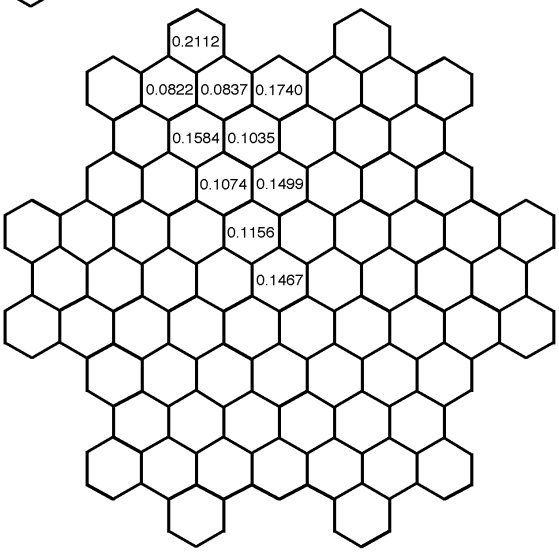

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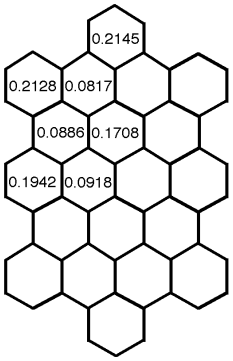

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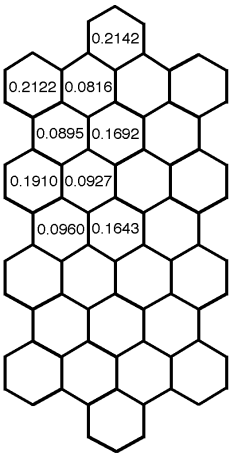

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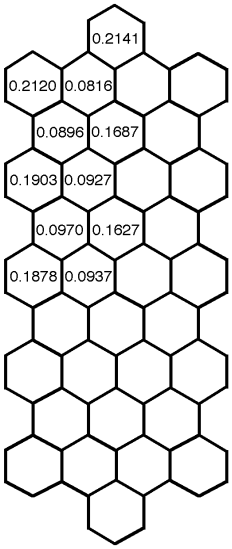

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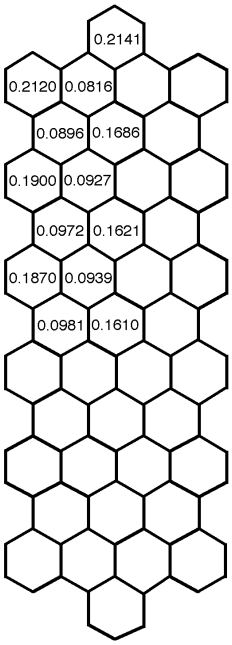

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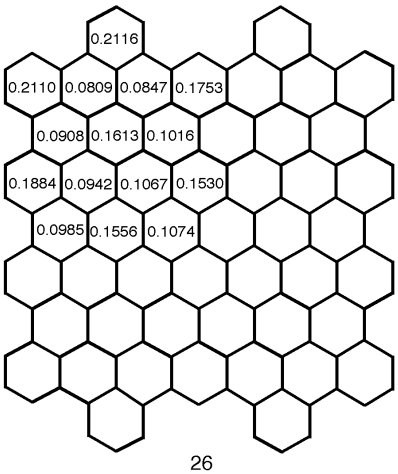

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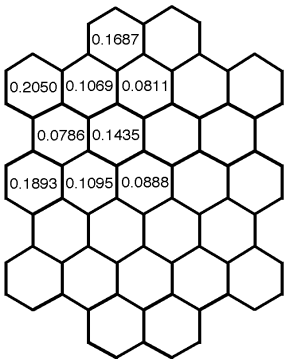

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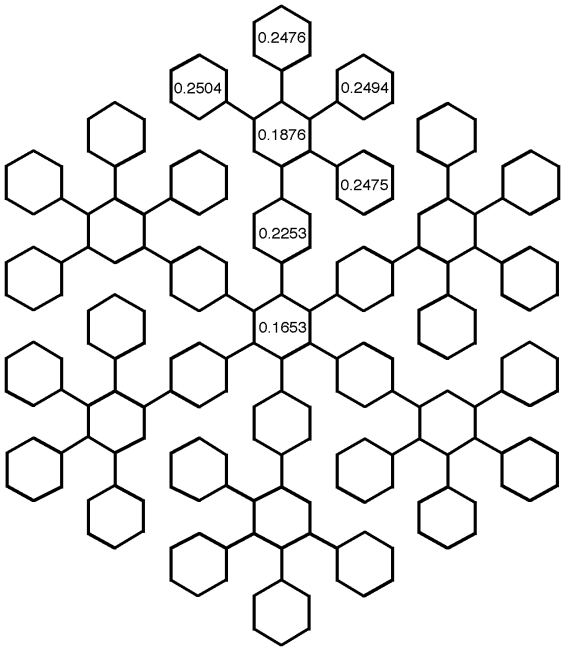
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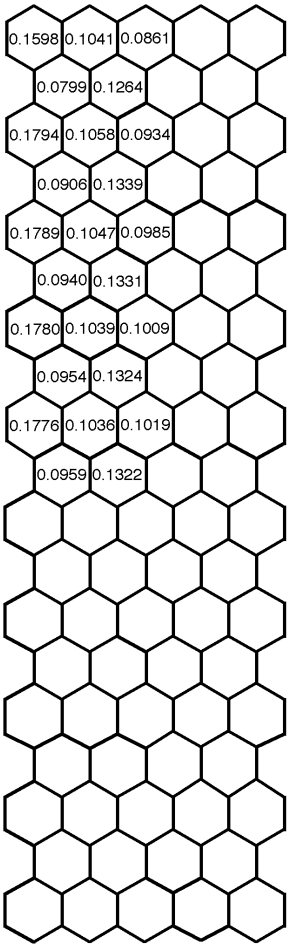
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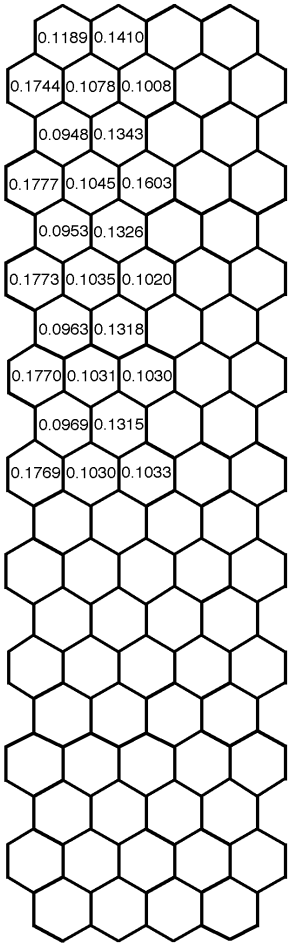
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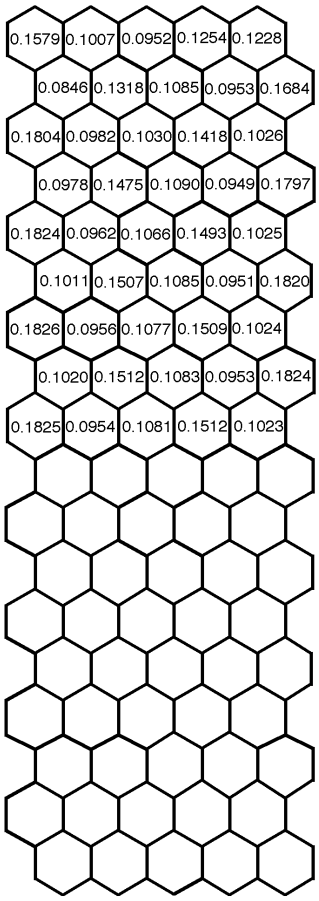
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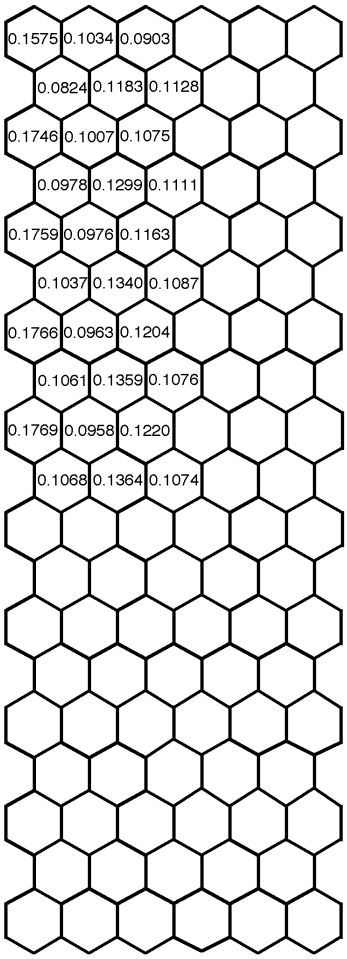
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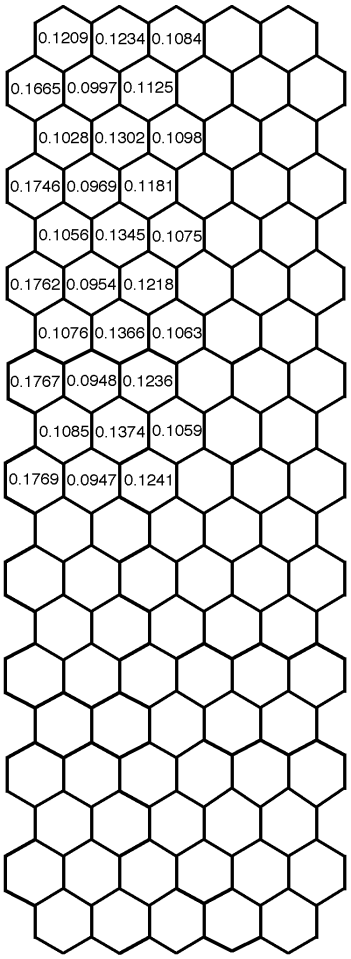
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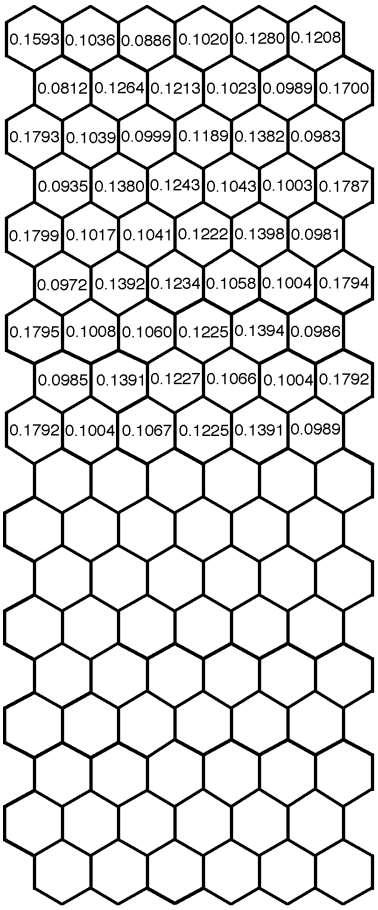
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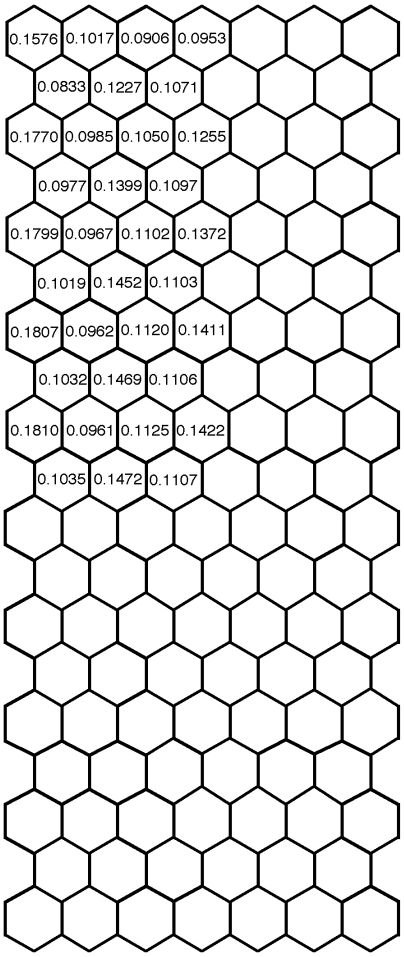
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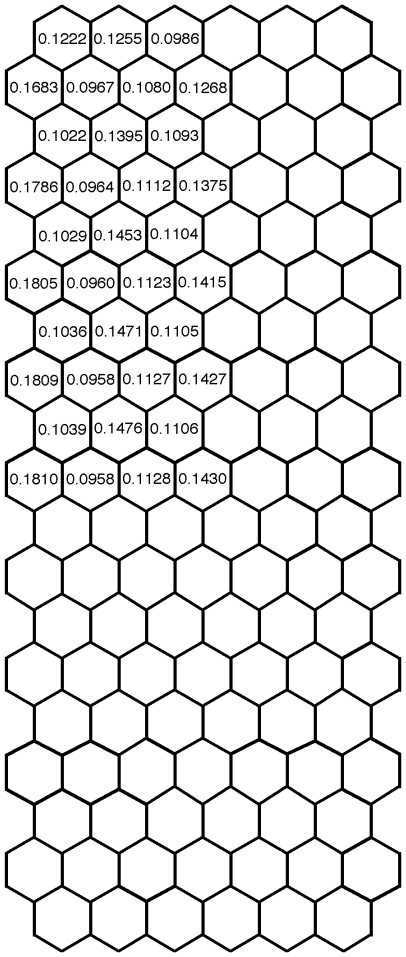
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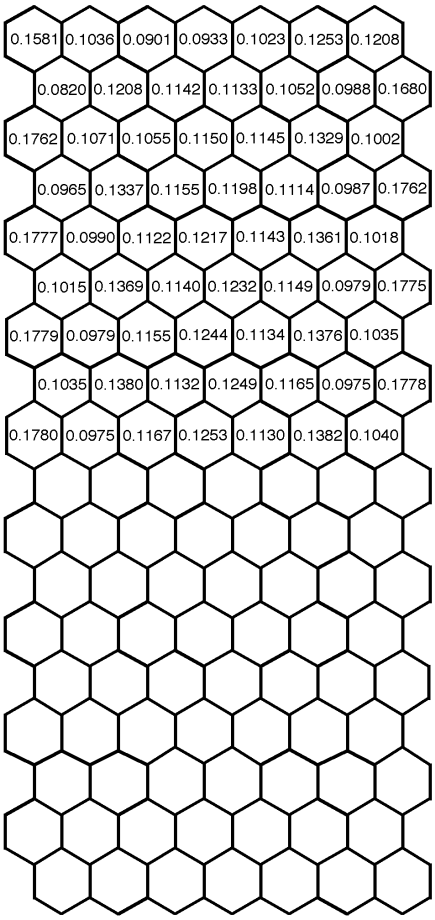
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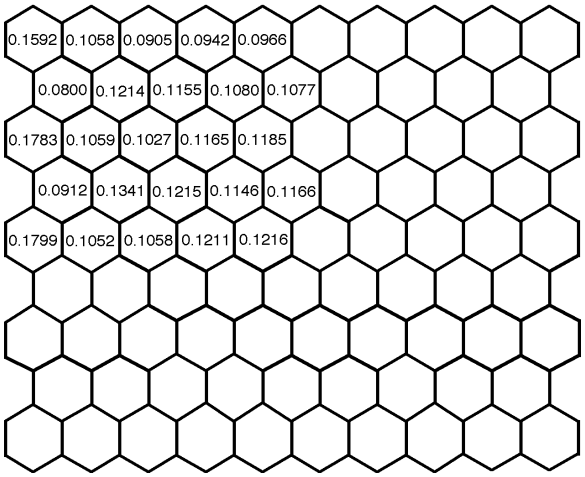
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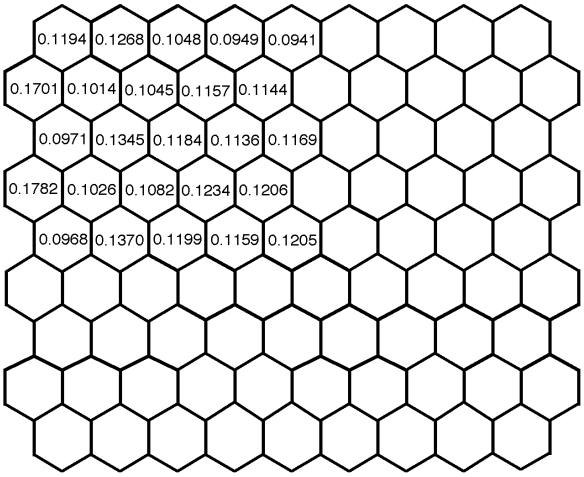
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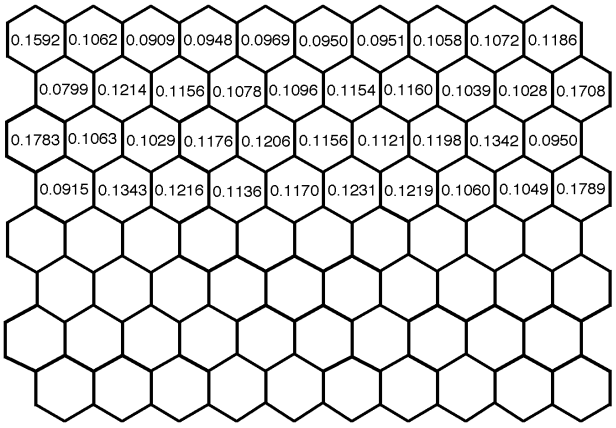
39


0.1592 0.1062 0.0909 0.0948 0.0969 0.0950 0.0951 0.1058 0.1072 0.1186
0.0799 0.1214 0.1156 0.1078 0.1096 0.1154 0.1160 0.1039 0.1028 0.1708
0.1783 0.1063 0.1029 0.1176 0.1206 0.1156 0.1121 0.1198 0.1342 0.0950
0.0915 0.1343 0.1216 0.1136 0.1170 0.1231 0.1219 0.1060 0.1049 0.1789

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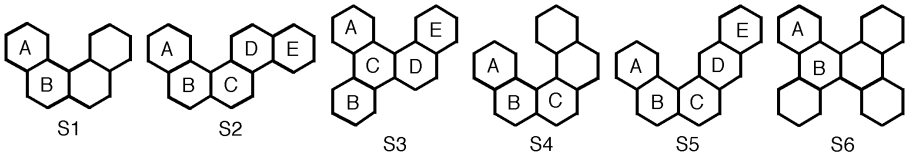
■ **Possible Correlation of SCI with SSE.**

A plot of the six-center index (SCI)[S3] against SSE for nonidentical benzene rings in benzene and 31 familiar PAHs is presented in Figures S1. We drew this figure using the SCI values calculated by Bultinck et al.[S3] at the B3LYP/6-31G* (6D,10F) level of theory and SSEs given in ref S1 and Table S1.

Table S1. SSEs and SCI Values for Benzene Rings in Six Familiar PAHs.



species	ring	SSE / $\lvert\beta\rvert$	SCI[a]
benzo[*c*]phenanthrene (**S1**)	A	0.2187	0.0298
	B	0.1578	0.0149
benzo[*c*]chrysene (**S2**)	A	0.2203	0.0304
	B	0.1513	0.0137
	C	0.1753	0.0186
	D	0.1496	0.0142
	E	0.2214	0.0299
benzo[*g*]chrysene (**S3**)	A	0.2298	0.0336
	B	0.2323	0.0336
	C	0.0983	0.0066
	D	0.1704	0.0169
	E	0.2149	0.0291
pentahelicene (**S4**)	A	0.2208	0.0304
	B	0.1499	0.0133
	C	0.1756	0.0186
naphth[1,2-*a*]anthracene (**S5**)	A	0.2156	0.0284
	B	0.1613	0.0162
	C	0.1268	0.0108
	D	0.1922	0.0197
	E	0.1820	0.0216
dibenzo[*g*,*p*]chrysene (**S6**)	A	0.2282	0.0329
	B	0.1087	0.0078

[a] Taken from ref S3.

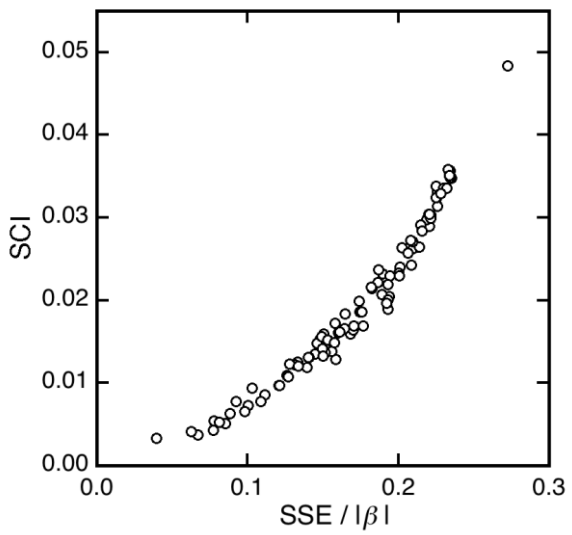


Figure S1. The SCI vs. SSE plot for all nonidentical rings in benzene and 31 familiar PAHs.

REFERENCES

(S1) Aihara, J.; Makino, M.; Sakamoto, K. Superaromatic Stabilization Energy as a Novel Local Aromaticity Index for Polycyclic Aromatic Hydrocarbons. *J. Phys. Chem. A*, **2013**, *117*, 10477-10488.

(S2) Aihara, J.; Makino, M. Constrained Clar Formulas of Coronoid Hydrocarbons. *J. Phys. Chem. A*, **2014**, *118*, 1258-1266.

(S3) Bultinck, P.; Ponec, R.; Van Damme, S. Multicenter Bond Indices as a New Measure of Aromaticity in Polycyclic Aromatic Hydrocarbons. *J. Phys. Org. Chem*. **2005**, *18*, 706-718.