SUPPLEMENTARY MATERIAL

Table 1 Aromaticity indices for all benzenoid rings in the PAH set. Molecule and ring labels are taken from table 1. For some indices literature values are used from the references cited. N/A means data not available in the cited paper.

Molecule	Ring	I_L	Z_L	Z_L^{π}	HOMA	BOIA	PDI	SCI	SCI$^{\pi}$	Ln(SCI)	FHDD	NICS	CRE[34]	RLHE[37]
1	1	1000	35.082	6.00	0.981	1.000	0.097	0.048	0.047	-3.04	1.000	-9.67	0.222	1000
2	1	912	34.404	5.65	0.767	0.981	0.067	0.026	0.025	-3.65	0.768	-9.99	0.112	945
3	1	893	34.339	5.56	0.616	0.966	0.057	0.020	0.019	-3.91	0.709	-8.84	0.090	934
3	2	840	33.778	5.39	0.690	0.979	0.061	0.019	0.017	-3.96	0.683	-12.60	0.063	902
4	1	888	34.314	5.52	0.527	0.958	0.053	0.017	0.016	-4.07	0.683	-7.83	0.086	930
4	2	825	33.731	5.32	0.600	0.972	0.058	0.016	0.014	-4.14	0.650	-12.59	0.052	890
5	1	886	34.302	5.51	0.479	0.954	0.050	0.016	0.015	-4.14	0.672	-7.06	N/A	930
5	2	821	33.713	5.29	0.535	0.968	0.056	0.014	0.013	-4.27	0.633	-12.05	N/A	888
5	3	811	33.689	5.27	0.550	0.969	0.057	0.014	0.013	-4.27	0.627	-13.49	N/A	881

6	1	888	34.297	5.50	0.453	0.952	0.049	0.015	0.014	-4.20	N/A	-6.53	N/A	930
6	2	824	33.704	5.28	0.498	0.965	0.055	0.014	0.012	-4.27	N/A	-11.44	N/A	888
6	3	816	33.674	5.24	0.505	0.966	0.057	0.013	0.012	-4.34	N/A	-13.50	N/A	879
7	1	885	34.295	5.50	0.438	0.950	0.049	0.015	0.014	-4.20	N/A	-6.05	N/A	N/A
7	2	819	33.700	5.28	0.475	0.963	0.054	0.013	0.012	-4.34	N/A	-10.85	N/A	N/A
7	3	806	33.667	5.23	0.475	0.964	0.056	0.012	0.011	-4.42	N/A	-13.18	N/A	N/A
7	4	804	33.660	5.22	0.467	0.964	0.057	0.012	0.011	-4.42	N/A	-13.94	N/A	N/A
8	1	928	34.497	5.74	0.854	0.990	0.073	0.031	0.030	-3.47	N/A	-10.06	0.141	956
8	2	813	33.713	5.26	0.433	0.953	0.039	0.012	0.012	-4.42	N/A	-6.81	0.052	885
9	1	882	34.174	5.57	0.830	0.987	0.059	0.024	0.024	-3.73	N/A	-12.75	0.099	929
9	2	818	33.771	5.29	0.553	0.956	0.035	0.012	0.012	-4.42	N/A	-5.09	0.051	889
10	1	923	34.485	5.73	0.832	0.988	0.071	0.030	0.029	-3.51	N/A	-9.95	0.132	952
10	2	832	33.806	5.37	0.542	0.963	0.045	0.015	0.015	-4.20	N/A	-7.69	0.066	896
11	1	940	34.589	5.82	0.886	0.994	0.076	0.035	0.034	-3.35	N/A	-9.00	0.165	963
11	2	714	33.002	4.87	0.044	0.926	0.024	0.005	0.005	-5.30	N/A	-2.82	0.024	821

12	1	899	34.357	5.59	0.697	0.973	0.060	0.022	0.021	-3.82	N/A	-9.31	N/A	937
12	2	850	33.846	5.46	0.729	0.980	0.060	0.021	0.019	-3.86	N/A	-11.69	N/A	908
12	3	793	33.642	5.16	0.268	0.940	0.031	0.009	0.008	-4.71	N/A	-4.59	N/A	872
12	4	930	34.516	5.77	0.883	0.993	0.075	0.033	0.032	-3.41	N/A	-9.81	N/A	957
13	1	837	33.884	5.39	0.713	0.970	0.044	0.016	0.016	-4.14	N/A	-11.03	0.067	N/A
13	2	753	33.232	5.08	0.597	0.947	0.033	0.008	0.008	-4.83	N/A	-1.24	0.030	N/A
14	1	913	34.447	5.68	0.768	0.982	0.065	0.026	0.025	-3.65	N/A	-10.45	N/A	946
14	2	795	33.501	5.24	0.575	0.964	0.044	0.013	0.013	-4.34	N/A	-11.16	N/A	875
14	3	802	33.714	5.21	0.427	0.946	0.028	0.009	0.009	-4.71	N/A	-2.42	N/A	880
14	4	838	33.875	5.40	0.644	0.967	0.044	0.016	0.015	-4.14	N/A	-6.50	N/A	899
14	5	880	34.178	5.57	0.827	0.987	0.058	0.024	0.023	-3.73	N/A	-12.06	N/A	927
15	1	929	34.511	5.76	0.873	0.992	0.074	0.032	0.031	-3.44	N/A	-9.93	N/A	N/A
15	2	800	33.661	5.19	0.355	0.945	0.033	0.010	0.009	-4.61	N/A	-5.39	N/A	N/A
15	3	863	33.919	5.54	0.789	0.984	0.062	0.023	0.021	-3.77	N/A	-11.27	N/A	N/A
16	1	929	34.510	5.76	0.870	0.992	0.074	0.032	0.031	-3.44	N/A	-9.87	N/A	N/A

16	2	800	33.669	5.19	0.346	0.945	0.033	0.010	0.009	-4.61	N/A	-5.38	N/A	N/A
16	3	863	33.916	5.54	0.791	0.983	0.061	0.023	0.021	-3.77	N/A	-11.28	N/A	N/A
17	1	940	34.589	5.82	0.889	0.994	0.077	0.035	0.034	-3.35	N/A	-8.63	N/A	962
17	2	720	33.048	4.90	0.179	0.929	0.024	0.005	0.006	-5.30	N/A	-1.18	N/A	825
17	3	894	34.267	5.64	0.838	0.989	0.062	0.027	0.026	-3.61	N/A	-11.58	N/A	934
17	4	818	33.769	5.28	0.516	0.954	0.036	0.012	0.012	-4.42	N/A	-5.46	N/A	888
18	1	890	34.325	5.54	0.570	0.962	0.054	0.018	0.017	-4.02	N/A	-8.37	N/A	N/A
18	2	829	33.740	5.34	0.657	0.975	0.058	0.017	0.015	-4.07	N/A	-12.62	N/A	N/A
18	3	834	33.790	5.39	0.611	0.969	0.054	0.017	0.015	-4.07	N/A	-11.00	N/A	N/A
18	4	787	33.614	5.11	0.183	0.934	0.027	0.007	0.007	-4.96	N/A	-3.27	N/A	N/A
18	5	931	34.520	5.78	0.893	0.994	0.075	0.034	0.033	-3.38	N/A	-9.53	N/A	N/A
19	1	901	34.366	5.60	0.725	0.976	0.061	0.023	0.022	-3.77	N/A	-9.37	N/A	N/A
19	2	851	33.854	5.47	0.733	0.979	0.058	0.021	0.019	-3.86	N/A	-10.98	N/A	N/A
19	3	772	33.570	5.05	0.117	0.929	0.023	0.006	0.006	-5.12	N/A	-2.23	N/A	N/A
20	1	903	34.364	5.60	0.738	0.975	0.061	0.023	0.022	-3.77	N/A	-9.05	N/A	N/A

20	2	859	33.918	5.51	0.768	0.979	0.060	0.022	0.020	-3.82	N/A	-10.39	N/A	N/A
20	3	694	32.936	4.77	-0.105	0.916	0.020	0.004	0.004	-5.52	N/A	-0.83	N/A	N/A
20	4	942	34.603	5.84	0.900	0.995	0.077	0.036	0.035	-3.32	N/A	-8.47	N/A	N/A
21	1	924	34.490	5.73	0.844	0.989	0.071	0.030	0.029	-3.51	N/A	-9.92	N/A	N/A
21	2	827	33.793	5.34	0.514	0.960	0.043	0.014	0.014	-4.27	N/A	-7.26	N/A	N/A
21	3	850	33.897	5.48	0.643	0.973	0.053	0.019	0.018	-3.96	N/A	-8.45	N/A	N/A
22	1	922	34.478	5.72	0.819	0.987	0.069	0.029	0.028	-3.54	N/A	-9.83	N/A	N/A
22	2	836	33.828	5.40	0.583	0.967	0.048	0.016	0.016	-4.14	N/A	-7.90	N/A	N/A
22	3	812	33.736	5.27	0.378	0.950	0.037	0.011	0.011	-4.51	N/A	-5.61	N/A	N/A
22	4	848	33.839	5.44	0.730	0.979	0.060	0.020	0.018	-3.91	N/A	-11.90	N/A	N/A
22	5	897	34.352	5.58	0.677	0.971	0.059	0.021	0.021	-3.86	N/A	-9.14	N/A	N/A
23	1	885	34.215	5.60	0.755	0.980	0.059	0.024	0.023	-3.73	N/A	-7.30	0.1012	929
23	2	698	32.940	4.77	-0.025	0.917	0.016	0.003	0.004	-5.81	N/A	6.64	0.022	814
24	1	940	34.588	5.82	0.895	0.994	0.076	0.035	0.034	-3.35	N/A	-8.64	N/A	N/A
24	2	719	33.041	4.89	0.139	0.926	0.024	0.005	0.005	-5.30	N/A	-1.55	N/A	N/A

24	3	906	34.364	5.71	0.843	0.990	0.065	0.029	0.028	-3.54	N/A	-10.42	N/A	N/A
25	1	941	34.603	5.83	0.903	0.995	0.077	0.036	0.035	-3.32	N/A	-8.06	N/A	N/A
25	2	704	32.993	4.82	0.059	0.921	0.020	0.004	0.004	-5.52	N/A	0.95	N/A	N/A
25	3	838	33.878	5.39	0.604	0.965	0.044	0.015	0.015	-4.20	N/A	-6.78	N/A	N/A
25	4	891	34.268	5.63	0.822	0.986	0.060	0.026	0.025	-3.65	N/A	-10.88	N/A	N/A
25	5	804	33.574	5.29	0.588	0.962	0.044	0.014	0.013	-4.27	N/A	-9.80	N/A	N/A
25	6	917	34.452	5.69	0.802	0.983	0.066	0.027	0.026	-3.61	N/A	-10.06	N/A	N/A
26	1	940	34.598	5.82	0.894	0.994	0.076	0.035	0.034	-3.35	N/A	-8.62	N/A	N/A
26	2	701	32.966	4.80	0.008	0.922	0.022	0.004	0.004	-5.52	N/A	-1.55	N/A	N/A
26	3	868	34.049	5.67	0.869	0.987	0.066	0.027	0.025	-3.61	N/A	-8.88	N/A	N/A

Supplementary Material for *Faraday Discussions*

COMPUTATIONAL DETAILS

For ab initio computed indices, molecular geometries were optimized at the B3LYP/6-31G* (6D,10F) level of theory using Gaussian-03. Own software was used for the computation of all indices. Some indices only have a meaning within the level of theory they were derived. In such case, either own software was developed to compute indices, or literature values were used.

In order to allow reproducing the data from tables 2-3, necessary details are given below:

- The DP index I_L is computed from Hückel MO theory using own Hückel software.
- NOEL indices Z_L are computed using B3LYP/6-31G* charge and bond order matrices. Geometries of the PAH are constructed from benzenoid rings with geometries exactly as in benzene. Hydrogen atoms are added with C-H bond lengths and valence angles as in benzene. π only values are reported as Z_L^{π}. Values are obtained using self-developed Molecular Quantum Similarity software.
- HOMA indices are computed using optimized B3LYP/6-31G* (6D,10F) geometries, using literature values for all constants. Calculations were performed using the self-developed Kekulé program.
- BOIA indices are computed using optimized B3LYP/6-31G* (6D,10F) geometries and Mulliken-like delocalization indices. B_0 values correspond to the

covalent delocalization indices in benzene. Calculations were performed using the self-developed Kekulé program.

- PDI indices are computed using optimized B3LYP/6-31G* (6D,10F) geometries and Mulliken-like delocalization indices. Calculations were performed using the self-developed Kekulé program.
- SCI values are computed using optimized B3LYP/6-31G* (6D,10F) geometries in the Mulliken approach to Generalized Population Analysis. π only values are reported as SCI^{π} . Calculations were performed using the self-developed Kekulé program.
- FHDD values ϑ are computed using corrected literature constants using optimized B3LYP/6-31G* (6D,10F) geometries and AIM delocalization indices. Calculations were performed using the self-developed Kekulé program.
- NICS values are computed using optimized B3LYP/6-31G* (6D,10F) geometries as NICS(0) isotropic values from Gaussian-03.
- Circuit Resonance Energies for benzenoid circuits are taken from the work of Aihara[34].
- Relative Local Hexagon Energies (RLHE) are taken from Valence Bond calculations of Jiang and Li[37].