J. Phys. Chem. A **2008,** *112,* 11769–11776 **11769**

A New Yardstick for Benzenoid Polycyclic Aromatic Hydrocarbons

Matevz Pompe[†]

Faculty of Chemistry and Chemical Technology, University of Ljubljana, Aškerčeva 5,
1001 Ljubljana, Slovenia

Milan Randić[‡]

National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia

Alexandru T. Balaban*

Texas A&M University at Galveston, 5007 Avenue U, Galveston, Texas 77551, and Visiting Scientist at the
Faculty of Chemistry and Chemical Technology, University of Ljubljana, Aškerčeva 5,
1001 Ljubljana, Slovenia

Received: June 7, 2008; Revised Manuscript Received: July 22, 2008

The newly introduced signature of benzenoids (a sequence of six real numbers s_i with $i = 6-1$) shows the composition of the π-electron partition by indicating the number of times all rings of the benzenoid are assigned 6, 5, 4, 3, 2, or 1 π-electrons. It allows the introduction of a new ordering criterion for such polycyclic aromatic hydrocarbons by summing some of the terms in the signature. There is an almost perfect linear correlation between sums $s_6 + s_5$ and $s_4 + s_3$ for isomeric cata- or peri-fused benzenoids, so that one can sort such isomers according to ascending $s_6 + s_5$ or to descending $s_4 + s_3$ sums (the resulting ordering does not differ much and agrees with that based on increasing numbers of Clar sextets and of Kekulé structures). Branched cata-condensed benzenoids have higher $s_6 + s_5$ sums than isomeric nonbranched systems. For nonisomeric peri-condensed benzenoids, both sums increase with increasing numbers of benzenoid rings and decrease with the number of internal carbon atoms. Other partial sums that have been explored are $s_6 + s_5 + s_3$ and $s_6 + s_2 + s_1$, and the last one appears to be more generally applicable as a parameter for the complexity of benzenoids and for ordering isomeric benzenoids.

Partition of π-Electrons in Rings of Benzenoids and Benzenoid Signatures

In a recent series of papers, the partition of π-electrons in rings of conjugated polycyclic hydrocarbons was discussed on the basis of the following convention: a shared C=C bond common to two condensed rings allows one π-electron to be assigned to each of these rings, whereas a nonshared C=C bond contributes with two π-electrons to the corresponding ring.[1−16] Upon counting for all resonance structures (assumed to have equal weights) how many π-electrons are assigned to each ring and upon dividing this count by the number K of resonance structures, one obtains the ring partition of all P π-electrons of the benzenoid.

For a given Kekuléan benzenoid, one can produce an array with h rows corresponding to each hexagonal ring showing the number of times each of the h benzenoid rings is assigned 6, 5, 4, 3, 2, 1, or 0 π-electrons on seven columns denoted by R_6 through R_0. The row sum divided by K provides the above-mentioned partition, but one can also look at the column sums (the R_i sequence of seven integers with $i = 6-0$). Obviously, $\sum_i R_i = Kh$. Upon dividing each R_i value by K, one obtains the r_i sequence with seven rational numbers, also with $i = 6-0$. Again, obviously, $\sum_i r_i = h$. The benzenoid signature (or the s_i sequence) is a sequence of six real numbers obtained from the r_i sequence by taking into account the number of π-electrons contributed by each of the h rings, $s_i = i \times r_i$; with the corollary, we arrive at the total number of π-electrons P from a different summation, namely, $P = \sum_i s_i$.[12−16] For catafusenes, $P = 4h + 2$, and for perifusenes $P = 4h - a + 2$ (where a denotes the number of internal carbon atoms).

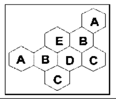
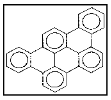
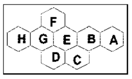
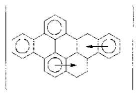
Ring	Partition	R_6	R_5	R_4	R_3	R_2	R_1	R_0	Ring denomination	Clar structure
2A	***5.33***	20	20	5	0	0	0	0		
2B	1.93	0	5	0	5	16	15	4		
2C	***4.80***	0	36	9	0	0	0	0		
D	1.73	0	0	4	4	17	16	4		
E	***4.13***	0	16	20	8	1	0	0		
	hK=360	**40**	**138**	**52**	**22**	**50**	**46**	**12**		
A	***4.97***	12	12	13	0	0	0	0		
B	3.70	0	11	9	12	5	0	0		
C	3.70	0	10	10	13	4	0	0		
D	***3.86***	0	10	14	11	2	0	0		
E	1.51	0	0	2	2	13	16	4		
F	***4.81***	0	30	7	0	0	0	0		
G	2.14	0	5	0	5	14	11	2		
H	***5.30***	16	16	5	0	0	0	0		
	hK=296	**28**	**94**	**60**	**43**	**38**	**27**	**6**		

Figure 1. The two isomeric octaperifusenes investigated by Clar and Zander, with their partitions and R_i sequences.

As an example, in Figure 1, one can see the corresponding partitions and R_i sequences, indicated in **boldface** characters in the last rows for each one of the two isomeric peri-condensed benzenoids with $h = 8$ (of Clar−Zander fame) having different reactivities.[17−19] Sums of entries in each row equal the number of resonance structures. One can observe that rings with Clar sextets have a higher value for the partition (***bold italic*** numbers)

---

[*] To whom correspondence should be addressed. E-mail: balabana@tamug.edu.

[†] E-mail: matevz.pompe@guest.arnes.si.

[‡] Visitor Emeritus, Department of Mathematics & Computer Science, Drake University, Des Moines, Iowa. E-mail: mrandic@msn.com.

10.1021/jp805020h CCC: $40.75

TABLE 1: Signatures and Partial Sums of Nonisoarithmic Catafusenes with $h = 2-6$ Benzenoid Rings

comp.	h	K	s_6	s_5	s_4	s_3	s_2	s_1	$s_6 + s_5$	$s_4 + s_3$	$s_2 + s_1$	s_{6521}	s_{621}	s_{653}
2c-1	2	3	4.000	3.333	2.667	0.000	0.000	0.000	7.333	2.667	0.000	7.333	4.000	7.333
3c-2	3	4	3.000	5.000	6.000	0.000	0.000	0.000	8.000	6.000	0.000	8.000	3.000	8.000
3c-3	3	5	6.000	4.000	2.400	1.200	0.400	0.000	10.000	3.600	0.400	10.400	6.400	11.200
4c-4	4	5	2.400	6.000	9.600	0.000	0.000	0.000	8.400	9.600	0.000	8.400	2.400	8.400
4c-5	4	7	5.143	6.429	4.571	1.286	0.571	0.000	11.572	5.857	0.571	12.143	5.714	12.858
4c-6	4	8	7.500	3.750	4.000	2.250	0.500	0.000	11.250	6.250	0.500	11.750	8.000	13.500
4c-7	4	9	8.667	6.667	1.333	0.333	0.667	0.333	15.334	1.666	1.000	16.334	9.667	15.667
5c-8	5	6	2.000	6.667	13.333	0.000	0.000	0.000	8.667	13.333	0.000	8.667	2.000	8.667
5c-9	5	9	4.667	7.778	7.556	1.333	0.667	0.000	12.445	8.889	0.667	13.112	5.334	13.778
5c-10	5	10	4.200	9.000	6.800	1.200	0.800	0.000	13.200	8.000	0.800	14.000	5.000	14.400
5c-11	5	11	6.545	5.909	6.545	2.455	0.545	0.000	12.454	9.000	0.545	12.999	7.090	14.909
5c-12	5	12	7.000	7.500	4.000	2.500	1.000	0.000	14.500	6.500	1.000	15.500	8.000	17.000
5c-13	5	13	9.231	3.846	4.923	3.231	0.769	0.000	13.077	8.154	0.769	13.846	10.000	16.308
5c-14	5	13	7.846	9.231	3.692	0.231	0.615	0.385	17.077	3.923	1.000	18.077	8.846	17.308
5c-15	5	14	9.857	6.071	3.429	1.500	0.857	0.286	15.928	4.929	1.143	17.071	11.000	17.428
6c-16	6	7	1.714	7.143	17.143	0.000	0.000	0.000	8.857	17.143	0.000	8.857	1.714	8.857
6c-17	6	11	4.364	8.636	10.909	1.364	0.727	0.000	13.000	12.273	0.727	13.727	5.091	14.364
6c-18	6	13	3.692	10.385	9.846	1.154	0.923	0.000	14.077	11.000	0.923	15.000	4.615	15.231
6c-19	6	14	6.000	7.143	9.714	2.571	0.571	0.000	13.143	12.285	0.571	13.714	6.571	15.714
6c-20	6	15	5.600	8.000	9.067	2.800	0.533	0.000	13.600	11.867	0.533	14.133	6.133	16.400
6c-21	6	16	6.750	9.375	6.000	2.625	1.250	0.000	16.125	8.625	1.250	17.375	8.000	18.750
6c-22	6	17	6.000	10.000	6.353	2.471	1.176	0.000	16.000	8.824	1.176	17.176	7.176	18.471
6c-23	6	17	7.412	10.588	6.824	0.176	0.588	0.412	18.000	7.000	1.000	19.000	8.412	18.176
6c-24	6	18	8.333	6.111	7.333	3.333	0.889	0.000	14.444	10.666	0.889	15.333	9.222	17.777
6c-25	6	19	8.526	7.105	5.684	3.632	1.053	0.000	15.631	9.316	1.053	16.684	9.579	19.263
6c-26	6	19	8.842	8.158	5.895	1.895	0.947	0.263	17.000	7.790	1.210	18.210	10.052	18.895
6c-27	6	19	6.947	11.842	6.105	0.158	0.526	0.421	18.789	6.263	0.947	19.736	7.894	18.947
6c-28	6	20	9.000	8.500	6.000	1.350	0.800	0.300	17.500	7.350	1.100	18.600	10.100	18.850
6c-29	6	21	10.857	3.810	6.095	4.286	0.952	0.000	14.667	10.381	0.952	15.619	11.809	18.953
6c-30	6	22	9.545	10.227	3.273	1.500	1.091	0.364	19.772	4.773	1.455	21.227	11.000	21.272
6c-31	6	22	11.182	5.682	5.091	2.727	1.091	0.227	16.864	7.818	1.318	18.182	12.500	19.591
6c-32	6	23	11.739	6.304	4.174	2.348	1.130	0.304	18.043	6.522	1.434	19.477	13.173	20.391
6c-33	6	24	12.000	8.333	2.667	1.000	1.500	0.500	20.333	3.667	2.000	22.333	14.000	21.333

than rings without Clar sextets. The first octaperifusene has $K = 45$ resonance structures and is a "sextet resonant benzenoid" with rings that either have a Clar sextet (indicated by the Armit−Robinson circle) or are "empty rings". With five Clar sextets, this benzenoid is unreactive toward dienophiles. By contrast, as shown by Clar and Zander,[17] the second benzenoid with $K = 37$ Kekulé valence structures has only four Clar sextets so that its Clar formula has also rings with conjugated double bonds and does react with dienophiles. The corresponding r_i and s_i sequences are 0.889, 3.067, 1.156, 0.489, 1.111, 1.033, 0.267 and 5.333, 15.333, 4.662, 1.467, 2.222, 1.022, respectively, for the first benzenoid with five Clar sextets and 0.757, 2.541, 1.622, 1.162, 1.027, 0.730, 0.162 and 4.541, 12.703, 6.486, 3.486, 2.054, 0.730, respectively, for the second benzenoid with four Clar sextets.

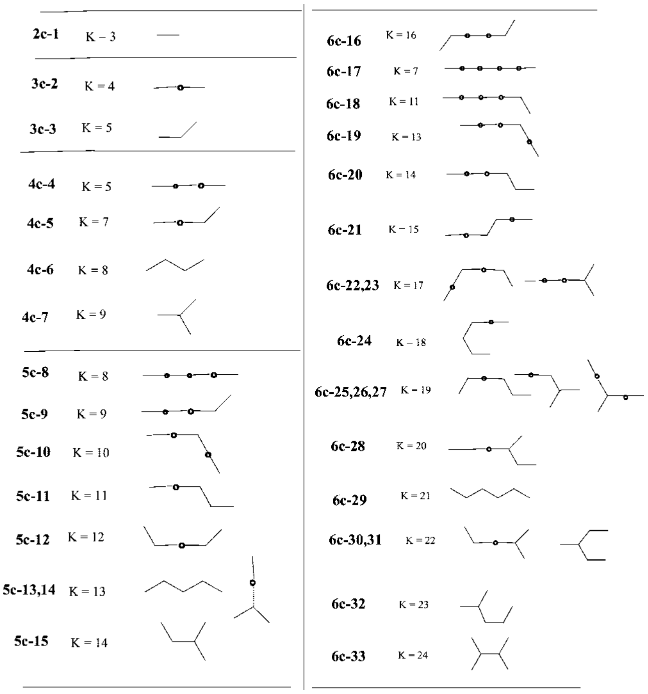


Figure 2. Dualists of catafusenes with $h = 2-6$ benzenoid rings. Isokekuléan (but not isoarithmic) benzenoids are on the same horizontal line.

We have investigated how to compress the information contained in the benzenoid signatures into a single number with low degeneracy that could serve as a parameter for expressing the complexity of a benzenoid and for ordering isomeric benzenoids. The simplest way for arriving at such a number is by means of partial sums of terms in the benzenoid signature. The number of Clar sextets and the number K of Kekulé valence structures (resonance structures) reflect the stability of benzenoids, but they are integers with high degeneracies. There is a correlation between these numbers manifested also in the fact that the number of Clar sextets is highest for fully resonant benzenoids among isomers; therefore, it should be sufficient to look at correlations with K for the targeted ordering parameter.

In several recent papers, the structures of cata- and pericondensed benzenoid with up to eight benzenoid rings were displayed.[1−16] Whenever the dualists of the benzenoids have notations that differ only in interchanging digits 1 and 2, most properties of such benzenoids (called isoarithmic benzenoids), including the number of resonance structures and the electron

TABLE 2: Signatures of Nonisoarithmic Heptacatafusenes and Their Partial Sums

no.	K	RE (eV)	s_6	s_5	s_4	s_3	s_2	s_1	s_{65}	s_{43}	s_{21}	s_{653}	s_{621}
7c-34	8	2.131	1.500	7.500	21.000	0.000	0.000	0.000	9.000	21.000	0.000	9.000	1.500
7c-35	13	2.900	4.154	9.231	14.462	1.385	0.769	0.000	13.385	15.846	0.769	14.770	4.923
7c-36	16	3.210	3.375	11.250	13.250	1.125	1.000	0.000	14.625	14.375	1.000	15.750	4.375
7c-38	17	3.279	5.647	7.941	13.176	2.647	0.588	0.000	13.588	15.824	0.588	16.235	6.235
7c-37	17	3.273	3.176	11.765	12.941	1.059	1.059	0.000	14.941	14.000	1.059	16.000	4.235
7c-39	19	3.279	5.053	9.211	12.210	3.000	0.526	0.000	14.263	15.210	0.526	17.264	5.579
7c-40	20	3.396	6.600	10.500	8.800	2.700	1.400	0.000	17.100	11.500	1.400	19.800	8.000
7c-42	22	3.562	5.455	11.364	9.454	2.455	1.273	0.000	16.818	11.909	1.273	19.274	6.728
7c-43	23	3.704	7.826	7.392	10.435	3.391	0.957	0.000	15.217	13.826	0.957	18.609	8.783
7c-44	23	3.734	5.739	11.957	8.348	2.478	1.478	0.000	17.696	10.826	1.478	20.174	7.217
7c-46	24	3.743	5.000	12.500	8.667	2.500	1.333	0.000	17.500	11.167	1.333	20.000	6.333
7c-48	25	3.857	7.440	8.400	9.760	3.360	1.040	0.000	15.840	13.120	1.040	19.200	8.480
7c-49	25	3.926	8.160	8.800	8.000	3.840	1.200	0.000	16.960	11.840	1.200	20.800	9.360
7c-51	26	3.898	7.615	9.231	8.154	3.923	1.077	0.000	16.846	12.077	1.077	20.769	8.692
7c-53	27	3.924	7.556	9.630	8.000	3.556	1.259	0.000	17.185	11.556	1.259	20.742	8.815
7c-56	29	4.030	9.931	6.035	8.552	4.448	1.034	0.000	15.966	13.000	1.034	20.414	10.965
7c-57	29	4.107	7.862	11.035	5.793	3.724	1.586	0.000	18.896	9.517	1.586	22.621	9.448
7c-59	30	4.199	10.000	6.667	7.467	4.800	1.067	0.000	16.667	12.267	1.067	21.467	11.067
7c-62	31	4.143	10.258	7.258	6.581	4.548	1.355	0.000	17.516	11.129	1.355	22.064	11.613
7c-70	34	4.238	12.529	3.824	7.176	5.294	1.176	0.000	16.353	12.471	1.176	21.647	13.705
7c-41	21	3.515	7.143	11.429	10.286	0.143	0.571	0.429	18.572	10.428	1.000	18.715	8.143
7c-45	24	3.722	8.250	9.375	9.000	2.125	1.000	0.250	17.625	11.125	1.250	19.750	9.500
7c-47	25	3.798	6.480	13.200	9.280	0.120	0.480	0.440	19.680	9.400	0.920	19.800	7.400
7c-50	26	3.831	8.539	9.808	9.231	1.269	0.769	0.385	18.346	10.500	1.154	19.616	9.693
7c-52	27	3.884	8.000	10.556	8.444	1.778	0.889	0.333	18.555	10.222	1.222	20.334	9.222
7c-54	28	3.983	6.000	14.465	8.572	0.107	0.429	0.429	20.465	8.679	0.857	20.572	6.858
7c-55	29	4.006	8.069	11.035	8.552	1.241	0.690	0.414	19.103	9.793	1.103	20.345	9.173
7c-58	30	4.038	10.200	7.834	7.467	3.100	1.200	0.200	18.034	10.567	1.400	21.134	11.600
7c-60	30	4.085	9.400	12.167	5.333	1.500	1.200	0.400	21.567	6.833	1.600	23.067	11.000
7c-61	31	4.089	10.258	7.903	8.000	2.516	1.032	0.290	18.161	10.516	1.323	20.677	11.580
7c-63	31	4.133	8.516	12.742	5.548	1.548	1.290	0.355	21.258	7.097	1.645	22.806	10.161
7c-64	32	4.146	10.875	8.594	6.625	2.344	1.250	0.313	19.469	8.969	1.563	21.813	12.438
7c-65	32	4.182	8.625	12.813	5.750	1.406	1.000	0.406	21.438	7.156	1.406	22.844	10.031
7c-66	33	4.211	10.909	8.788	6.667	2.182	1.091	0.364	19.697	8.849	1.455	21.879	12.364
7c-67	33	4.208	10.909	9.394	4.970	3.000	1.455	0.273	20.303	7.970	1.727	23.303	12.637
7c-68	34	4.255	10.765	11.030	4.941	1.765	1.176	0.324	21.794	6.706	1.500	23.560	12.265
7c-69	34	4.258	11.117	10.736	5.176	0.882	1.529	0.559	21.853	6.059	2.088	22.735	13.205
7c-71	35	4.277	12.686	5.572	6.172	4.029	1.371	0.171	18.257	10.200	1.543	22.287	14.228
7c-72	35	4.307	11.143	9.887	4.914	2.571	1.143	0.371	21.030	7.486	1.514	23.601	12.657
7c-73	36	4.329	13.000	5.834	6.000	3.583	1.333	0.257	18.834	9.583	1.590	22.417	14.590
7c-74	37	4.379	13.297	6.216	5.406	3.487	1.297	0.297	19.513	8.892	1.595	23.000	14.891
7c-75	38	4.411	13.421	8.027	4.210	2.210	1.684	0.447	21.447	6.421	2.132	23.658	15.552
7c-76	40	4.528	12.000	13.000	2.400	0.600	1.300	0.700	25.000	3.000	2.000	25.600	14.000
7c-77	41	4.557	14.341	8.781	3.512	1.317	1.415	0.634	23.122	4.829	2.049	24.439	16.390

distribution, are exactly the same. Therefore, for further discussions, we will examine only one of any set of isoarithmic benzenoids.

Starting with benzenoids with small numbers h of benzenoid rings, we present in Table 1 the signatures and partial sums of nonisoarithmic catafusenes with up to six benzenoid rings. The analogous Table 2 contains the same data for heptacatafusenes.[15,16] The notation for each compound contains (in boldface characters) the number of benzenoid rings followed by **c** for catafusenes and **p** for perifusenes, a hyphen, and a number that corresponds to the notation in previous papers that had presented structures, partitions, and sequences in detail.[15,16] In Table 3, we present signatures and partial sums for nonisoarithmic perifusenes with up to seven benzenoid rings having contiguous internal vertices. In the column labeled P of Tables 3 and 6, boldface numbers correspond to peri-condensed benzenoids having contiguous internal vertices. Their numbers of internal vertices are easily computed as $a = 4h + 2 - P$. Their molecular formula is C_PH_{P+2-2h}.

Figures 2 (catafusenes) and 3 (perifusenes) display structures of benzenoids with up to six benzenoid rings via their dualists, in which vertices correspond to centers of rings and edges connect vertices corresponding to condensed rings (i.e., rings sharing a CC bond). The ordering of structures in these figures and tables is first according to increasing h and then according to increasing K values. The structures and numbering of heptafusenes may be found in references published earlier.[15,16]

Properties of Partial Sums of Terms in Benzenoid Signatures

Among all possible partial sums of terms in benzenoid signatures, Tables 2 and 3 contain for each compound sums $s_6 + s_5$, $s_4 + s_3$, $s_2 + s_1$, $s_6 + s_5 + s_3$, and $s_6 + s_2 + s_1$ (denoted for brevity by s_{65}, s_{43}, s_{21}, s_{653}, and s_{621}, respectively). One can observe that whereas upon going from **6c-17** to **6c-33** or from **7p-19** to **7p-69**, s_{21} increases about twice and has small values, s_{65} and s_{43} have larger values, and s_{65} also increases about twice and s_{43} decreases about three times. Most interestingly, in a plot of these two last sums (s_{65} versus s_{43}) for catafusenes, there is an almost perfect linear correlation (for hexacatafusenes, the coefficient of determination is $R^2 = 0.998$), as seen in Figures 4 and 5. There is an explanation about this correlation, namely, the way that the P π-electrons are distributed. Of course, for a

TABLE 3: Signatures and Partial Sums of Perifusenes with $h = 4-7$ Benzenoid Rings

no.	h	K	s_6	s_5	s_4	s_3	s_2	s_1	P	s_{65}	s_{43}	s_{21}	s_{6521}	s_{653}	s_{621}
4p-1	4	6	0.000	8.333	4.000	3.000	0.667	0.000	16	8.333	7.000	0.667	9.000	11.333	0.667
5p-2	5	9	0.000	13.333	5.333	0.000	0.889	0.444	20	13.333	5.333	1.333	14.666	13.333	1.333
5p-3	5	9	2.000	7.778	5.333	4.000	0.889	0.000	20	9.778	9.333	0.889	10.667	13.778	2.889
5p-4	5	11	2.727	10.909	3.273	1.636	1.091	0.364	20	13.636	4.909	1.455	15.091	15.272	4.182
6p-5	6	9	0.000	13.333	5.333	4.000	1.333	0.000	24	13.333	9.333	1.333	14.666	17.333	1.333
6p-6	6	10	0.000	7.000	7.200	6.600	1.200	0.000	**22**	7.000	13.800	1.200	8.200	13.600	1.200
6p-7	6	12	1.500	11.667	8.667	0.750	1.000	0.417	24	13.167	9.417	1.417	14.584	13.917	2.917
6p-8	6	12	1.500	9.583	7.667	4.250	1.000	0.000	24	11.083	11.917	1.000	12.083	15.333	2.500
6p-9	6	13	3.692	6.923	7.385	5.077	0.923	0.000	24	10.615	12.462	0.923	11.538	15.692	4.615
6p-10	6	14	4.286	7.500	6.000	4.929	1.286	0.000	24	11.786	10.929	1.286	13.072	16.715	5.572
6p-11	6	14	0.000	10.714	5.714	3.643	1.571	0.357	**22**	10.714	9.357	1.928	12.642	14.357	1.928
6p-12	6	15	2.400	13.667	5.067	1.200	1.200	0.467	24	16.067	6.267	1.667	17.734	17.267	4.067
6p-13	6	15	3.600	8.333	5.867	5.000	1.200	0.000	24	11.933	10.867	1.200	13.133	16.933	4.800
6p-14	6	16	4.500	10.000	5.000	2.813	1.375	0.313	24	14.500	7.813	1.688	16.188	17.313	6.188
6p-15	6	16	1.875	13.438	5.750	1.500	1.000	0.438	24	15.313	7.250	1.438	16.751	16.813	3.313
6p-16	6	17	3.882	10.294	5.412	2.824	1.294	0.294	24	14.176	8.236	1.588	15.764	17.000	5.470
6p-17	6	17	4.941	10.294	4.706	2.471	1.176	0.412	24	15.235	7.177	1.588	16.823	17.706	6.529
6p-18	6	20	5.400	13.500	2.400	0.600	1.400	0.700	**24**	18.900	3.000	2.100	21.000	19.500	7.500
7p-19	7	9	0.000	13.333	9.333	4.000	1.333	0.000	28	13.333	13.333	1.333	14.666	17.333	1.333
7p-20	7	12	1.500	11.667	8.667	5.000	1.167	0.000	28	13.167	13.667	1.167	14.334	18.167	2.667
7p-21	7	14	1.714	6.429	8.857	7.714	1.286	0.000	**26**	8.143	16.571	1.286	9.429	15.857	3.000
7p-22	7	15	2.400	13.667	5.067	5.000	1.867	0.000	28	16.067	10.067	1.867	17.934	21.067	4.267
7p-23	7	15	2.400	10.667	12.267	1.200	1.067	0.400	28	13.067	13.467	1.467	14.534	14.267	3.867
7p-24	7	15	1.200	12.667	11.467	1.200	1.067	0.400	28	13.867	12.667	1.467	15.334	15.067	2.667
7p-25	7	15	1.200	10.667	10.667	4.400	1.067	0.000	28	11.867	15.067	1.067	12.934	16.267	2.267
7p-26	7	16	3.000	10.000	12.000	1.500	1.125	0.375	28	13.000	13.500	1.500	14.500	14.500	4.500
7p-27	7	16	2.250	6.875	7.750	7.500	1.625	0.000	**26**	9.125	15.250	1.625	10.750	16.625	3.875
7p-28	7	17	3.176	8.529	9.882	5.471	0.941	0.000	28	11.705	15.353	0.941	12.646	17.176	4.117
7p-29	7	18	0.000	10.000	7.111	7.333	1.556	0.000	**26**	10.000	14.444	1.556	11.556	17.333	1.556
7p-30	7	18	0.000	12.500	8.000	3.500	1.556	0.444	**26**	12.500	11.500	2.000	14.500	16.000	2.000
7p-31	7	19	3.789	10.000	7.579	5.053	1.579	0.000	28	13.789	12.632	1.579	15.368	18.842	5.368
7p-32	7	19	2.842	9.474	6.947	4.737	1.579	0.421	**26**	12.316	11.684	2.000	14.316	17.053	4.842
7p-33	7	20	1.800	9.500	7.800	4.800	1.800	0.300	**26**	11.300	12.600	2.100	13.400	16.100	3.900
7p-34	7	20	3.900	12.000	8.400	1.950	1.300	0.450	28	15.900	10.350	1.750	17.650	17.850	5.650
7p-35	7	20	0.000	7.500	7.200	6.900	2.100	0.300	**24**	7.500	14.100	2.400	9.900	14.400	2.400
7p-36	7	21	4.286	12.381	7.238	2.143	1.524	0.429	28	16.667	9.381	1.953	18.620	18.810	6.239
7p-37	7	21	3.429	13.095	7.810	1.714	1.524	0.429	28	16.524	9.524	1.953	18.477	18.238	5.382
7p-38	7	21	1.714	15.952	7.238	1.286	1.333	0.476	28	17.666	8.524	1.809	19.475	18.952	3.523
7p-39	7	21	2.571	10.714	8.381	5.000	1.333	0.000	28	13.285	13.381	1.333	14.618	18.285	3.904
7p-40	7	21	3.429	10.952	6.667	5.429	1.524	0.000	28	14.381	12.096	1.524	15.905	19.810	4.953
7p-41	7	21	4.000	11.667	7.238	3.286	1.524	0.286	28	15.667	10.524	1.810	17.477	18.953	5.810
7p-42	7	21	1.429	14.762	8.952	1.429	0.952	0.476	28	16.191	10.381	1.428	17.619	17.620	2.857
7p-43	7	22	5.455	7.727	7.455	6.000	1.364	0.000	28	13.182	13.455	1.364	14.546	19.182	6.819
7p-44	7	22	2.182	10.455	6.727	4.500	1.727	0.409	**26**	12.637	11.227	2.136	14.773	17.137	4.318
7p-45	7	23	5.739	7.826	6.957	6.000	1.478	0.000	28	13.565	12.957	1.478	15.043	19.565	7.217
7p-46	7	23	4.435	12.174	7.130	2.609	1.217	0.435	28	16.609	9.739	1.652	18.261	19.218	6.087
7p-47	7	23	3.652	12.391	7.826	2.348	1.391	0.391	28	16.043	10.174	1.782	17.825	18.391	5.434
7p-48	7	23	2.870	12.391	7.826	3.261	1.391	0.261	28	15.261	11.087	1.652	16.913	18.522	4.522
7p-49	7	23	2.348	12.391	5.739	3.000	1.913	0.609	**26**	14.739	8.739	2.522	17.261	17.739	4.870
7p-50	7	24	4.500	12.917	6.667	2.250	1.167	0.500	28	17.417	8.917	1.667	19.084	19.667	6.167
7p-51	7	24	3.750	13.542	6.667	2.250	1.333	0.458	28	17.292	8.917	1.791	19.083	19.542	5.541
7p-52	7	24	5.250	8.125	7.167	6.125	1.333	0.000	28	13.375	13.292	1.333	14.708	19.500	6.583
7p-53	7	24	6.500	9.167	7.000	3.625	1.333	0.375	28	15.667	10.625	1.708	17.375	19.292	8.208
7p-54	7	24	6.500	9.167	6.333	4.000	1.750	0.250	28	15.667	10.333	2.000	17.667	19.667	8.500
7p-55	7	25	4.800	14.000	4.800	2.400	1.520	0.480	28	18.800	7.200	2.000	20.800	21.200	6.800
7p-56	7	25	5.760	9.600	6.720	4.080	1.600	0.240	28	15.360	10.800	1.840	17.200	19.440	7.600
7p-57	7	25	4.080	12.800	7.200	2.400	1.040	0.480	28	16.880	9.600	1.520	18.400	19.280	5.600
7p-58	7	25	2.640	13.000	5.120	2.640	1.920	0.680	**26**	15.640	7.760	2.600	18.240	18.280	5.240
7p-59	7	26	6.000	9.615	7.231	3.462	1.308	0.385	28	15.615	10.693	1.693	17.308	19.077	7.693
7p-60	7	27	7.333	10.000	5.481	3.333	1.407	0.444	28	17.333	8.814	1.851	19.184	20.666	9.184
7p-61	7	27	6.222	10.741	5.333	3.667	1.704	0.333	28	16.963	9.000	2.037	19.000	20.630	8.259
7p-62	7	27	6.000	10.926	5.333	4.000	1.407	0.333	28	16.926	9.333	1.740	18.666	20.926	7.740
7p-63	7	27	3.556	14.444	5.333	2.778	1.481	0.407	28	18.000	8.111	1.888	19.888	20.778	5.444
7p-64	7	28	5.786	10.536	6.143	3.643	1.571	0.321	28	16.322	9.786	1.892	18.214	19.965	7.678
7p-65	7	28	6.429	10.714	5.429	3.536	1.500	0.393	28	17.143	8.965	1.893	19.036	20.679	8.322
7p-66	7	29	6.000	12.586	4.552	2.379	2.000	0.483	28	18.586	6.931	2.483	21.069	20.965	8.483
7p-67	7	29	4.552	16.034	4.828	0.517	1.310	0.759	28	20.586	5.345	2.069	22.655	21.103	6.621
7p-68	7	30	7.400	12.500	4.267	1.600	1.533	0.700	28	19.900	5.867	2.233	22.133	21.500	9.633
7p-69	7	31	6.581	12.903	4.387	1.935	1.548	0.645	28	19.484	6.322	2.193	21.677	21.419	8.774

plot of s_{6521} versus s_{43}, one would have a perfect correlation with $R^2 = -1$ because $s_{6521} + s_{43} = P$, the number of all π-electrons. Then, one has to consider that s_{21} adds a relatively small contribution to s_{65}.

Such linear correlations between sums $s_6 + s_5$ and $s_4 + s_3$ are general, and they occur on practically parallel lines that depend on the number of rings (and for perifusenes, also on the number of internal vertices). As illustrated, Figure 4 presents

TABLE 4: Correlation Coefficient *R* between *K* Values and Partial Sums of Signature Terms

	7-cata-all	7-cata-br.	7-cata-nonbr.	7-peri-all	7-peri-2-int.	7-peri-4-int.	8-peri-4-int.
$s_6 = -s_{54321}$	0.940	0.889	0.926	0.777	0.813	0.538	0.485
$s_5 = -s_{64321}$	−0.161	−0.369	−0.361	0.205	0.043	0.804	0.815
$s_4 = -s_{65321}$	−0.935	−0.916	−0.916	−0.764	−0.786	−0.728	−0.922
$s_3 = -s_{65421}$	0.237	0.394	0.939	−0.348	−0.190	−0.849	−0.867
$s_2 = -s_{65431}$	0.610	0.778	0.678	0.273	0.450	0.027	0.786
$s_1 = -s_{65432}$	0.620	0.293	–	0.592	0.579	0.797	0.892
$s_{21} = -s_{6543}$	0.821	0.831	0.678	0.559	0.685	0.503	0.947
$s_{31} = -s_{6542}$	0.364	0.164	0.939	−0.304	−0.120	−0.851	−0.859
$s_{41} = -s_{6532}$	−0.927	−0.917	−0.916	−0.720	−0.748	−0.601	−0.885
$s_{51} = -s_{6432}$	−0.102	−0.344	−0.361	0.248	0.099	0.816	0.830
$s_{61} = -s_{5432}$	0.946	0.900	0.926	0.812	0.847	0.631	0.623
$s_{32} = -s_{6541}$	0.346	0.523	0.972	−0.293	−0.115	−0.840	−0.828
$s_{42} = -s_{6531}$	−0.941	−0.904	−0.928	−0.788	−0.299	−0.801	−0.902
$s_{52} = -s_{6431-}$	−0.072	−0.281	−0.235	0.238	0.094	−0.801	0.842
$s_{62} = -s_{5431}$	0.943	0.889	0.950	0.799	0.821	0.568	0.585
$s_{43} = -s_{6521}$	−0.850	−0.696	−0.778	−0.788	−0.755	−0.910	−0.953
$s_{53} = -s_{6421}$	−0.036	−0.294	0.250	−0.117	−0.133	0.150	0.383
$s_{63} = -s_{5421}$	0.849	0.799	0.936	0.402	0.493	−0.530	−0.539
$s_{54} = -s_{6321}$	−0.876	−0.824	−0.953	−0.377	−0.587	0.629	0.370
$s_{64} = -s_{5321}$	−0.154	0.111	−0.331	0.092	−0.040	0.036	−0.687
$s_{65} = -s_{4321}$	0.837	0.628	0.790	0.780	0.745	0.940	0.948
$s_{321} = -s_{654}$	0.459	0.582	0.971	−0.244	−0.036	−0.838	−0.812
$s_{421} = -s_{653}$	−0.935	−0.909	−0.928	−0.743	−0.760	−0.669	−0.854
$s_{521} = -s_{643}$	−0.016	−0.256	−0.235	0.280	0.146	0.811	0.854
$s_{621} = -s_{543}$	**0.951**	**0.900**	**0.950**	**0.832**	**0.853**	**0.657**	**0.695**
$s_{431} = -s_{652}$	−0.853	−0.711	−0.778	−0.780	−0.758	−0.916	−0.957
$s_{531} = -s_{642}$	0.041	−0.263	0.250	−0.025	−0.047	0.323	0.576
$s_{631} = -s_{542}$	0.872	0.817	0.937	0.471	0.557	−0.474	−0.461
$s_{541} = -s_{652}$	−0.854	−0.808	−0.930	−0.318	−0.527	0.667	0.462
$s_{641} = -s_{532}$	−0.083	0.140	−0.331	0.163	0.039	0.175	−0.545
$s_{651} = -s_{432}$	0.831	0.615	0.790	0.716	0.743	0.934	0.945

an analogous correlation for catafusenes with $h = 2-6$, and Figure 5 displays the same correlation for hexaperifusenes (only the upper points of the preceding figure). In Figure 4, one can recognize the four parallel directions corresponding to the benzenoids with $h = 3-6$. In Figure 6, one can see the many points corresponding to hexaperifusenes with two internal vertices and two points on a parallel direction for the two hexaperifusenes with four internal vertices, namely **6p-6** and **6p-11**.

There is also segregation according to whether the catafusene has a branched dualist or a nonbranched dualist. As one can see in Figure 7A and B, the nonbranched catafusenes are concentrated in the upper left part of the straight line, whereas the branched isomers are concentrated on the lower left end of the same line.

Correlations between Numbers *K* of Resonance Structures and Partial Sums of Signature Terms

We have explored the correlation between *K* values and all possible partial sums of terms in the signatures of representative sets of benzenoids, having a sufficient number of isomeric compounds in each set. For the set of catafusenes with seven benzenoid rings, Table 4 presents selections from the Pearson product-moment correlation coefficient *R* for single, pair, and triplet sums. One should take into account the equality (with changed *R* sign) between the 15 pair sums and the quadruplet sums, as well as that between half of the 20 triplet sums and the remaining half. Because for nonbranched catafusenes all s_1 terms are zero, there is no number in the corresponding site of Table 4. A relatively small set of perifusenes with eight benzenoid rings and four internal contiguous vertices is also included in Table 4.

It can be seen that the *R* values for singlets s_6, s_2, and s_1 are always positive, for s_4, they are always negative, and for s_5 and s_3, they change sign upon passing from catafusenes to perifusenes. Among doublet sums, s_{21}, s_{61}, s_{62}, and s_{65} lead always to positive *R* values, s_{41}, s_{42}, and s_{43} lead to negative *R* values, and other doublet sums cause sign changes. One can understand these observations by remembering that s_6 and s_4 (with opposite signs) have larger values than other partial sums, whereas s_1, s_2, s_3, and s_5 have relatively smaller values.

Another conclusion based on looking at the entries in Table 4 (any heptacatafusene and heptaperifusenes with less than four internal carbon atoms) is that the triplet sum $s_6 + s_2 + s_1$ (denoted as s_{621} for brevity, and similarly for other partial sums) with boldface entries in Table 4 can be considered to be the most general parameter for the complexity of all benzenoids, although for certain other sets of isomeric compounds, other partial sums (such as s_{65} or s_{653}) may yield higher correlation coefficients.

Correlations between Resonance Energies and Partial Sums of Signature Terms

In addition to numbers of Clar structures or resonance structures, a more refined and less degenerate property of benzenoids is the resonance energy (RE). There are several types and corresponding programs for obtaining resonance energy values.

In Table 2, one can see the RE values (in eV) for heptacatafusenes calculated according to the conjugated circuits method.[20] For all nonisoarithmic heptacatafusenes, there is an excellent correlation between RE and ln *K* values,[21] as seen in Figure 8. Upon plotting RE values for all (except the three least and most branched ones **7c-34**, **7c-41**, and **7c-70)** heptacatafusenes against partial sums of signature terms s_{621} (Figure 9) and s_{653} (Figure 10), satisfactory correlations are obtained. Although the latter is slightly better than the former, taking into

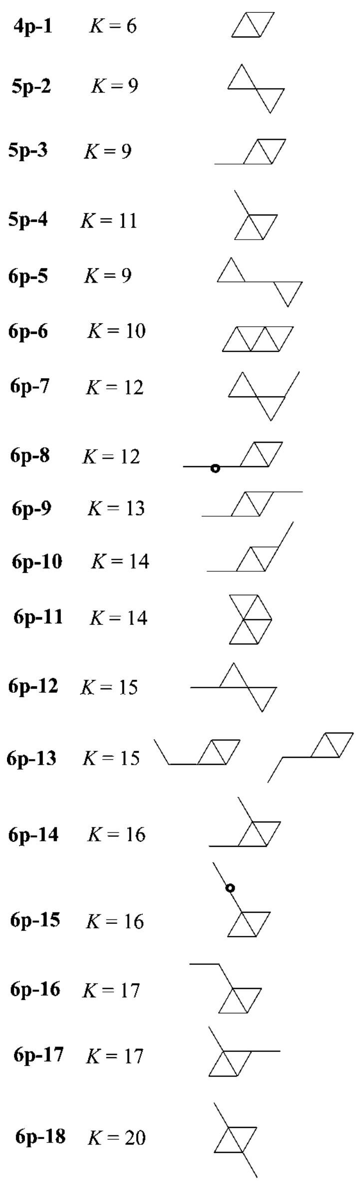


Figure 3. Dualists of perifusenes with $h = 4-6$ benzenoid rings. Isoarithmic benzenoids are on the same horizontal line.

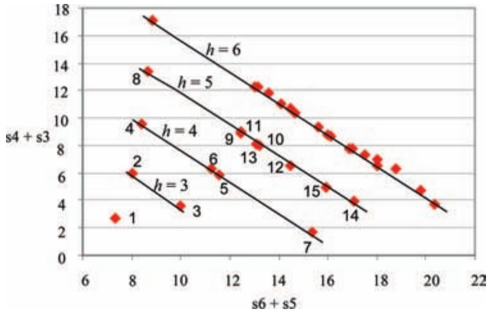


Figure 4. Plot of sums $s_3 + s_4$ versus $s_5 + s_6$ for catafusenes with $h = 2-6$ carbon atoms. In Figure 2, the benzenoids were denoted by ***h*c-*x***, but here, they are indicated only by ***x*** for $h = 2-5$.

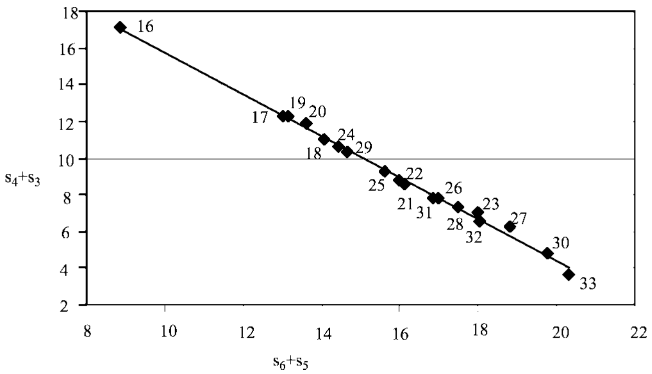


Figure 5. Plot of $s_4 + s_3$ versus $s_6 + s_5$ for hexacatafusenes indicated in Figure 2 by **6c-*x*** and here by ***x*** ($R^2 = 0.9962$, $y = 27.122 - 1.1357x$).

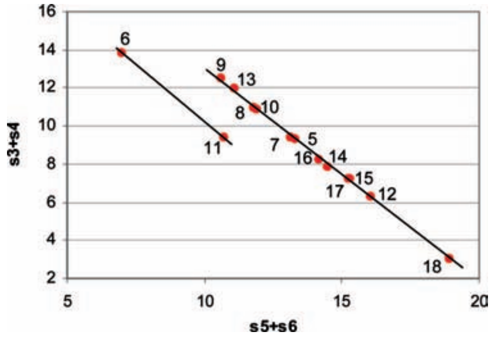


Figure 6. Plot of sums $s_4 + s_3$ versus $s_6 + s_5$ for hexaperifusenes indicated in Figure 3 by **6p-*x*** and here by ***x***.

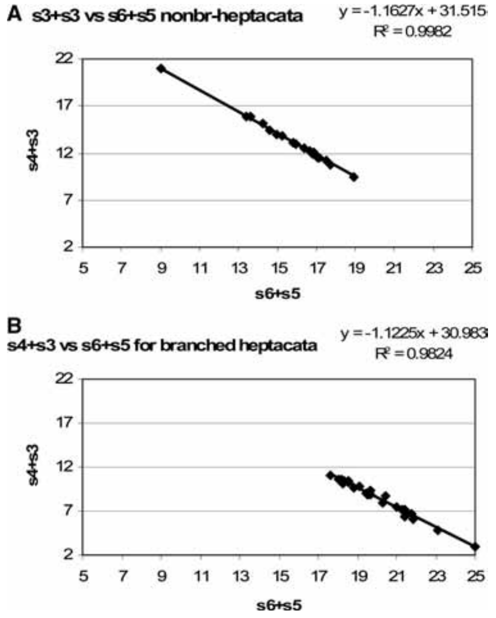


Figure 7. Plots of sums $s_3 + s_4$ versus $s_5 + s_6$ for nonbranched (A, upper part) and branched heptacatafusenes (B, lower part).

account the information of the preceding section, we will concentrate henceforth on s_{621} as the preferred ordering parameter.

A Novel Yardstick and the Corresponding Ordering of Benzenoids

In a previous paper,[13] for the set of all 33 possible nonisoarithmic octaperifusenes with four contiguous internal vertices, the ordering induced by s_{6521} or s_{652} was found to approximate fairly well that induced by K values; the partial sum s_{621} did not lead to satisfactory results. It was mentioned there that for catafusenes, the latter parameter provided better results than the two former ones. In the present paper, we are now able to substantiate this claim, concentrating on s_{621}.

Among the various partial sums indicated in Table 4, we have to choose one to encode the complexity of benzenoids and to allow an ordering of isomeric benzenoids. The chosen parameter

TABLE 5: Heptacatafusenes Ordered by s_{621} (Separately for Nonbranched and Branched)

no.	K	$s_6 + s_5$	$s_4 + s_3$	$s_2 + s_1$	$s_6 + s_2 + s_1$
7c-34	8	9.000	21.000	0.000	1.500
7c-37	17	14.941	14.000	1.059	4.235
7c-36	16	14.625	14.375	1.000	4.375
7c-35	13	13.385	15.846	0.769	4.923
7c-39	19	14.263	15.210	0.526	5.579
7c-38	17	13.588	15.824	0.588	6.235
7c-46	24	17.500	11.167	1.333	6.333
7c-42	22	16.818	11.909	1.273	6.728
7c-44	23	17.696	10.826	1.478	7.217
7c-40	20	17.100	11.500	1.400	8.000
7c-48	25	15.840	13.120	1.040	8.480
7c-51	26	16.846	12.077	1.077	8.692
7c-43	23	15.217	13.826	0.957	8.783
7c-53	27	17.185	11.556	1.259	8.815
7c-49	25	16.960	11.840	1.200	9.360
7c-57	29	18.896	9.517	1.586	9.448
7c-56	29	15.966	13.000	1.034	10.965
7c-59	30	16.667	12.267	1.067	11.067
7c-62	31	17.516	11.129	1.355	11.613
7c-70	34	16.353	12.471	1.176	13.705
7c-54	28	20.465	8.679	0.857	6.858
7c-47	25	19.680	9.400	0.920	7.400
7c-41	21	18.572	10.428	1.000	8.143
7c-55	29	19.103	9.793	1.103	9.173
7c-52	27	18.555	10.222	1.222	9.222
7c-45	24	17.625	11.125	1.250	9.500
7c-50	26	18.346	10.500	1.154	9.693
7c-65	32	21.438	7.156	1.406	10.031
7c-63	31	21.258	7.097	1.645	10.161
7c-60	30	21.567	6.833	1.600	11.000
7c-61	31	18.161	10.516	1.323	11.580
7c-58	30	18.034	10.567	1.400	11.600
7c-68	34	21.794	6.706	1.500	12.265
7c-66	33	19.697	8.849	1.455	12.364
7c-64	32	19.469	8.969	1.563	12.438
7c-67	33	20.303	7.970	1.727	12.637
7c-72	35	21.030	7.486	1.514	12.657
7c-69	34	21.853	6.059	2.088	13.205
7c-76	40	25.000	3.000	2.000	14.000
7c-71	35	18.257	10.200	1.543	14.228
7c-73	36	18.834	9.583	1.590	14.590
7c-74	37	19.513	8.892	1.595	14.891
7c-75	38	21.447	6.421	2.132	15.552
7c-77	41	23.122	4.829	2.049	16.390

must be general, even if it is not always the one with the highest correlation coefficient with K or RE.

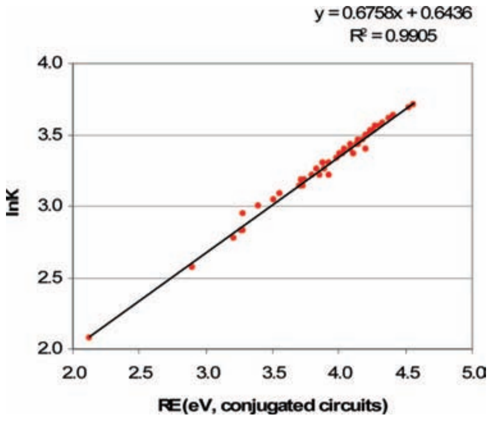


Figure 8. Plot of ln K versus resonance energies (RE in eV) for all nonisoarithmic heptacatafusenes.

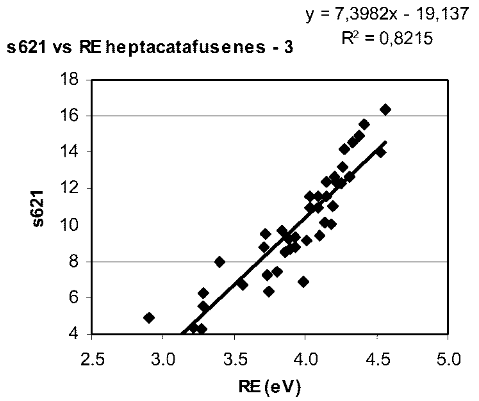


Figure 9. Plot of sum s_{621} versus RE for all but three nonisoarithmic heptacatafusenes.

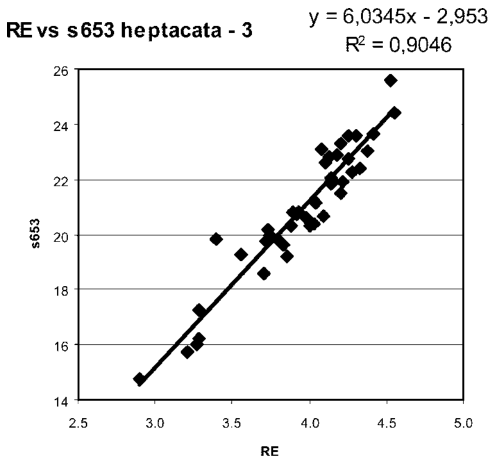


Figure 10. Plot of sum s_{653} versus RE for all but three nonisoarithmic heptacatafusenes.

In Table 4, one sees that the sum of terms $s_6 + s_2 + s_1$ (s_{621}), which is displayed in boldface characters, looks to be the best choice because it always affords positive correlation coefficients with K, and in most cases, it has the highest R values. Now for looking at the ordering induced by this parameter, let us consider Tables 5 and 6 with cata- and peri-condensed heptafusenes. For nonbranched heptacatafusenes, shown in the first half of Table 5, it can be observed that the ordering induced by s_{621} does not differ much from that induced by K; it does, however, differ a little more for branched catafusenes shown in the second half of Table 5. Also, the ordering of heptaperifusenes induced by s_{621} differs fairly frequently from that induced by K, but the general trends with the lowest and highest values are not different in any of the systems examined.

In Tables 3 and 6, one may observe for compounds **7p-20** and **7p-24** the first case of degeneracy among partial sums for terms in signatures. Such degeneracies are to be expected because the terms in signatures are rational numbers; therefore, degeneracies may occur for some combinations of s_i terms.

Conclusions

A study is presented on how to compress into one index of complexity the benzenoid signatures, which represent the sequence of six rational numbers into which the number P of π-electrons is divided in nonisoarithmic cata- and peri-condensed Kekuléan benzenoids. Partial sums of terms in benzenoid signatures may serve as parameters for characterizing the complexity of benzenoids. It was found that the Pearson correlation coefficients R with the number K of resonance structures are always positive for terms s_6, s_2, and s_1 of the signature; for s_4, they are always negative, and for s_5 and s_3,

TABLE 6: Perifusenes Ordered by *h* and Then by s_{621}

no.	h	K	P	s_{65}	s_{43}	s_{21}	s_{621}
4p-1	4	6	16	8.333	7.000	0.667	0.667
5p-2	5	9	20	13.333	5.333	1.333	1.333
5p-3	5	9	20	9.778	9.333	0.889	2.889
5p-4	5	11	20	13.636	4.909	1.455	4.182
6p-6	6	10	**22**	7.000	13.800	1.200	1.200
6p-5	6	9	24	13.333	9.333	1.333	1.333
6p-11	6	14	**22**	10.714	9.357	1.929	1.928
6p-8	6	12	24	11.083	11.917	1.000	2.500
6p-7	6	12	24	13.167	9.417	1.417	2.917
6p-15	6	16	24	15.313	7.250	1.438	3.313
6p-12	6	15	24	16.067	6.267	1.667	4.067
6p-9	6	13	24	10.615	12.462	0.923	4.615
6p-13	6	15	24	11.933	10.867	1.200	4.800
6p-16	6	17	24	14.176	8.235	1.588	5.470
6p-10	6	14	24	11.786	10.929	1.286	5.572
6p-14	6	16	24	14.500	7.813	1.688	6.188
6p-17	6	17	24	15.235	7.176	1.588	6.529
6p-18	6	20	24	18.900	3.000	2.100	7.500
7p-19	7	9	28	13.333	13.333	1.333	1.333
7p-29	7	18	**26**	10.000	14.444	1.556	1.556
7p-30	7	18	**26**	12.500	11.500	2.000	2.000
7p-25	7	15	28	11.867	15.067	1.067	2.267
7p-35	7	20	**24**	7.500	14.100	2.400	2.400
7p-20	7	12	28	13.167	13.667	1.167	2.667
7p-24	7	15	28	13.867	12.667	1.467	2.667
7p-42	7	21	28	16.190	10.381	1.429	2.857
7p-21	7	14	**26**	8.143	16.571	1.286	3.000
7p-38	7	21	28	17.667	8.524	1.810	3.523
7p-23	7	15	28	13.067	13.467	1.467	3.867
7p-27	7	16	**26**	9.125	15.250	1.625	3.875
7p-33	7	20	**26**	11.300	12.600	2.100	3.900
7p-39	7	21	28	13.286	13.381	1.333	3.904
7p-28	7	17	28	11.706	15.353	0.941	4.117
7p-22	7	15	28	16.067	10.067	1.867	4.267
7p-44	7	22	**26**	12.636	11.227	2.136	4.318
7p-26	7	16	28	13.000	13.500	1.500	4.500
7p-48	7	23	28	15.261	11.087	1.652	4.522
7p-32	7	19	**26**	12.316	11.684	2.000	4.842
7p-49	7	23	**26**	14.739	8.739	2.522	4.870
7p-40	7	21	28	14.381	12.095	1.524	4.953
7p-58	7	25	**26**	15.640	7.760	2.600	5.240
7p-31	7	19	28	13.789	12.632	1.579	5.368
7p-37	7	21	28	16.524	9.524	1.952	5.382
7p-47	7	23	28	16.043	10.174	1.783	5.434
7p-63	7	27	28	18.000	8.111	1.889	5.444
7p-51	7	24	28	17.292	8.917	1.792	5.541
7p-57	7	25	28	16.880	9.600	1.520	5.600
7p-34	7	20	28	15.900	10.350	1.750	5.650
7p-41	7	21	28	15.667	10.524	1.810	5.810
7p-46	7	23	28	16.609	9.739	1.652	6.087
7p-50	7	24	28	17.417	8.917	1.667	6.167
7p-36	7	21	28	16.667	9.381	1.952	6.239
7p-52	7	24	28	13.375	13.292	1.333	6.583
7p-67	7	29	28	20.586	5.345	2.069	6.621
7p-55	7	25	28	18.800	7.200	2.000	6.800
7p-43	7	22	28	13.182	13.455	1.364	6.819
7p-45	7	23	28	13.565	12.957	1.478	7.217
7p-56	7	25	28	15.360	10.800	1.840	7.600
7p-64	7	28	28	16.321	9.786	1.893	7.678
7p-59	7	26	28	15.615	10.692	1.692	7.693
7p-62	7	27	28	16.926	9.333	1.741	7.740
7p-53	7	24	28	15.667	10.625	1.708	8.208
7p-61	7	27	28	16.963	9.000	2.037	8.259
7p-65	7	28	28	17.143	8.964	1.893	8.322
7p-66	7	29	28	18.586	6.931	2.483	8.483
7p-54	7	24	28	15.667	10.333	2.000	8.500
7p-69	7	31	28	19.484	6.323	2.194	8.774
7p-60	7	27	28	17.333	8.815	1.852	9.184
7p-68	7	30	28	19.900	5.867	2.233	9.633

they change sign upon passing from catafusenes to perifusenes. Upon searching all such possible partial sums for cata- and peri-condensed benzenoids with up to seven benzenoid rings, it was observed that plots of pairwise sums $s_6 + s_5$ versus $s_4 + s_3$ afford linear correlations with intercepts depending on the branching of catafusenes and on the numbers of internal vertices for perifusenes. Among all other partial sums, it appears that s_{621}, that is, $s_6 + s_2 + s_1$, represents the best parameter for this purpose because it presents a satisfactory correlation with the number K of Kekulé structures (and therefore also with the number of Clar sextets). Among all benzenoids with up to seven benzenoid rings, only one pair of heptaperifusenes with the same value for this parameter was found.

Acknowledgment. The authors acknowledge the financial support of the Slovenian Research Agency through the Research Grants P1-0153, BI-US/06-07-025 and 1000-07-780002, of the Slovenian Human Resources Development and Scholarship Ad-Futura.

References and Notes

(1) Randić, M.; Balaban, A. T. Partitioning of π-electrons in rings of polycyclic conjugated hydrocarbons. Part 1. Catacondensed benzenoids. *Polycyclic Aromat. Compd.* **2004**, *24*, 173–193.

(2) Balaban, A. T.; Randić, M. Partitioning of π-electrons in rings of polycyclic benzenoid hydrocarbons. Part 2. Catacondensed coronoids. *J. Chem. Inf. Comput. Sci.* **2004**, *44*, 50–59.

(3) Balaban, A. T.; Randić, M. Partitioning of π-electrons in rings of polycyclic conjugated hydrocarbons. Part 3. Perifusenes. *New J. Chem.* **2004**, *28*, 800–806.

(4) Vukičević, D.; Randić, M.; Balaban, A. T. Partitioning of π-electrons in rings of polycyclic conjugated hydrocarbons. Part 4. Benzenoids with more than one geometric Kekule structure corresponding to the same algebraic Kekulé structure. *J. Math. Chem.* **2004**, *36*, 271–279.

(5) Balaban, A. T.; Randić, M. Partitioning of π-electrons in rings of polycyclic conjugated hydrocarbons. Part 5. Nonalternant compounds. *J. Chem. Inf. Comput. Sci.* **2004**, *44*, 1701–1707.

(6) Gutman, I.; Randić, M.; Balaban, A. T.; Furtula, B.; Vučković, V. π-Electron contents of rings in the double-hexagonal chain homologous series (pyrene, anthanthrene and other acenoacenes). *Polycyclic Aromat. Compd.* **2005**, *25*, 215–226.

(7) Randič, M.; Balaban, A. T. Partitioning of -electrons in rings for Clar structures of benzenoid hydrocarbons. *J. Chem. Inf. Model.* **2006**, *46*, 57–64.

(8) Balaban, A. T.; Furtula, B.; Gutman, I.; Kovačević, R. Partitioning of π-electrons in rings of aza-derivatives of polycyclic benzenoid hydrocarbons. *Polycyclic Aromat. Compd.* **2007**, *27*, 51–63.

(9) Balaban, A. T.; Randič, M. Partitioning of π-electrons in rings of polycyclic conjugated hydrocarbons. Part 6. Comparison with other methods for estimating the local aromaticity of rings in polycyclic benzenoids. *J. Math. Chem.* **2005**, *37*, 443–453.

(10) Balaban, A. T.; Gutman, I.; Stanković, S. Effect of heteroatoms on partitioning of π-electrons in rings of catafusenes. *Polycyclic Aromat. Compd.* **2008**, *28*, 85–97.

(11) Balaban, A. T.; Randić, M.; Vukičević, D. Partition of π-electrons between faces of polyhedral carbon aggregates. *J. Math. Chem.* **2008**, *43*, 773–779.

(12) Balaban, A. T.; Randić, M. Perfect matchings in polyhexes, or recent graph-theoretical contributions to benzenoids. *J. Univers. Comput. Sci.* **2007**, *13*, 1514–1539.

(13) Balaban, A. T.; Randić, M.; Pompe, M. π-Electron partitions, signatures, and Clar structures of selected benzenoid hydrocarbons. *J. Phys. Chem. A* **2008**, *112*, 4148–4157.

(14) Balaban, A. T.; Randić, M. Correlations between various ways of accounting for the distribution of π-electrons in benzenoids. *New J. Chem.* **2008**, *32*, 1071–1078.

(15) A. T., Balaban.; Randić, M. Ring signatures for benzenoids with up to seven rings. Part 1. *cata*-Condensed systems. *Int. J. Quantum Chem.* **2008**, *108*, 865–897.

(16) Balaban, A. T.; Randić, M. Ring signatures for benzenoids with up to seven rings. Part 2. peri-Condensed systems. *Int. J. Quantum Chem.* **2008**, *108*, 898–926.

(17) Clar, E.; Zander, M. 1:12−2:3−10:11-Tribenzoperylene. *J. Chem. Soc.* **1958**, 1861–1865.

(18) Clar, E. *The Aromatic Sextet*; Wiley: London, 1972.

(19) Dias, J. R. *Handbook of Polycyclic Hydrocarbons, Part A. Benzenoid Hydrocarbons*; Elsevier: Amsterdam, 1987.

(20) Randić, M. Aromaticity of polycyclic conjugated hydrocarbons. *Chem. Rev.* **2003**, *103*, 3449–3606.

(21) Swinborne-Sheldrake, R.; Herndon, W. C.; Gutman, I. *Tetrahedron Lett.* **1975**, *16*, 755–758.

JP805020H