π-Electron Partitions, Signatures, and Clar Structures of Selected Benzenoid Hydrocarbons

Alexandru T. Balaban*,†

Texas A&M University at Galveston, 5007 Avenue U, Galveston, Texas 77551

Matevž Pompe‡

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

Milan Randić§

National Institute of Chemistry, Hajdrihova 19, SI-1001 Ljubljana, Slovenia

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It is shown for a representative set of isomeric benzenoids that π-electron partitions and signatures can serve for characterizing and ordering benzenoids. Benzenoid signatures (sequences s_6 through s_1 where the subscripts correspond to numbers of π electrons in all rings) are obtained by examining the numbers of assigned π electrons ranging from 6 to 1 for each ring in all resonance structures. The π-electron partitions and signatures of all 33 non-isoarithmic *peri*-condensed benzenoid hydrocarbons with eight rings and four contiguous internal carbon atoms allow an ordering of these benzenoids that agrees fairly well with increasing numbers of Kekulé valence structures and Clar sextets. Interestingly, an excellent correlation ($R^2 > 0.99$) is observed between $s_6 + s_5 + s_2 + s_1$ and $s_4 + s_3$, and an explanation for this observation is provided: the number P of π electrons is divided unequally between two components: $s_{34} = s_4 + s_3$ and $s_{1256} = s_6 + s_5 + s_2 + s_1$ so that s_{1256} or the quotient $s_{1256}/s_{34} = Q$ can serve *as* a new metric for perfect matchings of polyhexes and a criterion for ordering and for evaluating the complexity of isomeric benzenoids quantitatively.

Introduction

On the basis of all resonance structures of a benzenoid and the convention to assign to each ring two or one π electrons for each non-shared or shared C═C bond, respectively,[1,2] a series of articles examined the resulting π-electron partitions of various types of benzenoids and related conjugated hydrocarbons.[3−20] Recently, an extension of this examination led to “benzenoid signatures”, namely sequences s_6 through s_1 where the subscripts correspond to numbers of π electrons in all rings.[21−23]

peri-Condensed benzenoids (perifusenes) are polycyclic benzenoid hydrocarbons with internal carbon atoms, or equivalently their dualists (inner dual graphs) have three-membered rings. Although all *cata*-condensed benzenoids (catafusenes) with the same number h of hexagonal rings are isomeric, this is not the case for perifusenes. Their molecular formulas also depend on the number a of internal carbon atoms. An h ring benzenoid’s molecular formula C_nH_{n+2-2h} indicates that it contains $n = 4h + 2 - a$ carbon atoms and $2h + 4 - a$ hydrogen atoms.

The structures of benzenoids are mirrored in the geometry of their dualists consisting of vertices (centers of hexagons) and edges connecting vertices corresponding of hexagons sharing a CC bond. For *cata*-fused benzenoids, the dualists are acyclic, whereas for *peri*-fused ones they have triangles. Structural codes use digit 0 for denoting a straight annelation as in acenes, and digits 1 or 2 for “kinked” annelation as in the middle ring of phenanthrene. A canonical code has the minimal number formed by digits when starting from one end of the catafusene; the same digit must always denote the same direction of a kink (either left or right).[24,25] Acenes have codes consisting only of zeros, and the numbers K of their resonance structures are $K = h + 1$. When there is no zero in the code, the benzenoid is a fibonacene because it has a Fibonacci number as K.[26−29] In the definition of benzenoids one can include helicenes, which are fibonacenes, or one may exclude them because their carbon scaffolds are not fragments of a graphene sheet.

When codes of catafusenes differ only by interconversion of digits 1 and 2, the corresponding benzenoids have the same K values and there are one-to-one correspondences between their resonance structures; therefore, all of their electronic properties are quite similar. Such catafusenes (or catafusene fragments) are called isoarithmic.[30] For example all fibonacenes, whose structural codes have no digit 0 (cata-condensed benzenoids with no anthracenic subgraphs, such as helicenes encoded by sequences of digit 1, or zigzag catafusenes encoded by alternating sequences of digits 1 and 2) are isoarithmic.

Octaperifusenes with Four Contiguous Internal Carbon Atoms

We have selected a representative set of kekuléan *peri*-condensed benzenoids that have contiguous internal vertices (essentially disconnected benzenoids such as perylene or zethrene have noncontiguous internal vertices) and nonzero K values. These polycyclic aromatic hydrocarbons are truly delocalized benzenoids. There are 33 possible non-isoarithmic octaperi-

* Corresponding author. E-mail: balabana@tamug.edu.
† Visiting scientist at the University of Ljubljana, Faculty of Chemistry and Chemical Technology.
‡ E-mail: matevz.pompe@guest.arnes.si.
§ Emeritus, Department of Mathematics and Computer Science, Drake University, Des Moines, IA. E-mail: mrandic@msn.com.

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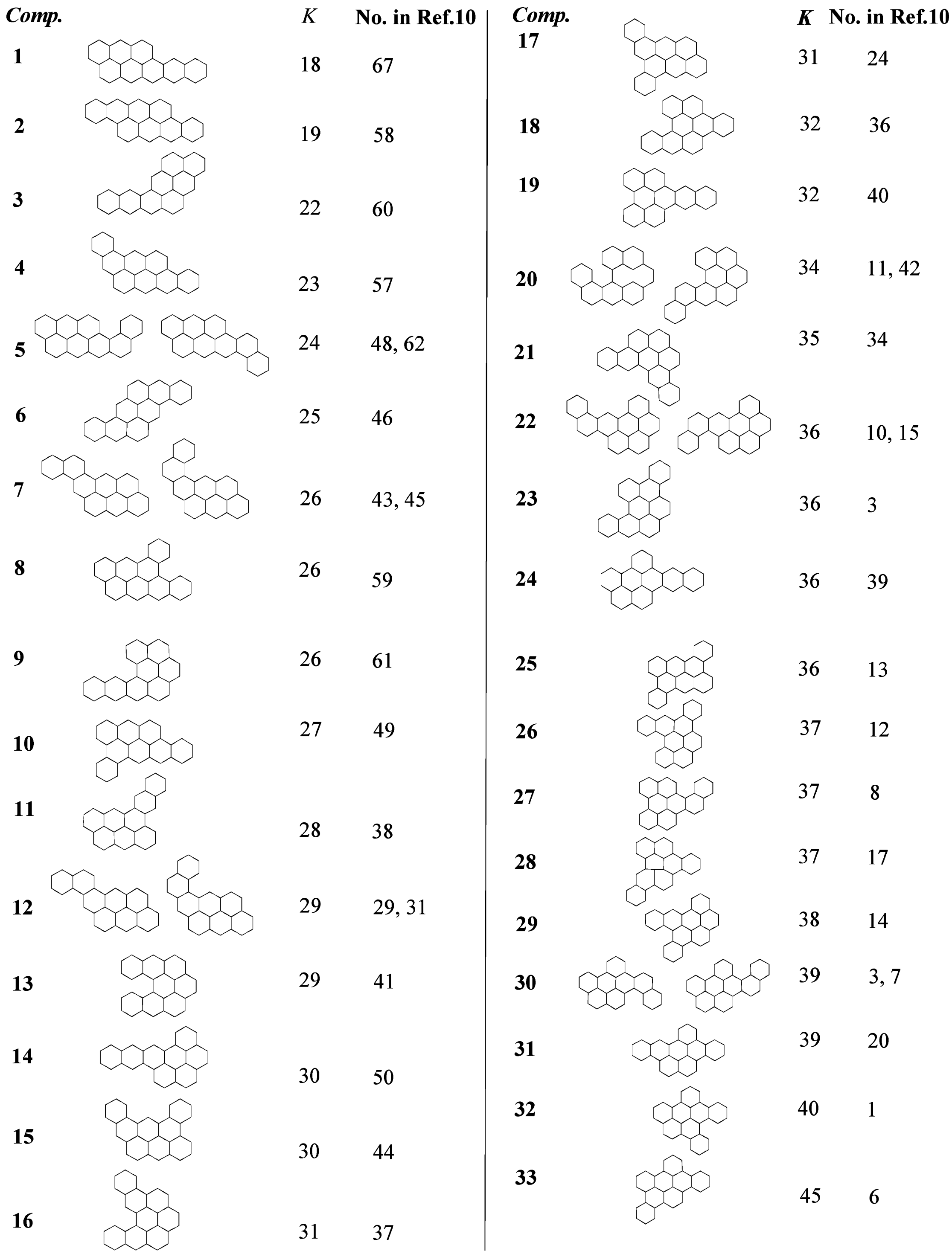


Figure 1. All 39 possible octaperifusenes with four contiguous internal vertices. Isoarithmic ones are on the same line so that there are 33 non-isoarithmic octaperifusenes **1**−**33**. They are presented with their K values and the coding given in the book by Knop et al.

fusenes ($h = 8$) with four contiguous internal carbon atoms ($a = 4$), indicated in Figure 1. In the book by Knop, Müller, Szymanski, and Trinajstić,[31] structures of all benzenoids with up to nine benzenoid rings are indicated with a code containing three numbers separated by full stops: number h of benzenoid rings, number a of internal carbon atoms, and an arbitrary ordering number, x. The 39 octaperifusenes with four internal carbon atoms are denoted by 8.4.x in the above-mentioned book.[31] In Figure 1, only the last of these numbers (x) is indicated for each benzenoid. Six of these benzenoids have each one isoarithmic isomer, as shown in Table 1, namely **5**, **7**, **12**, **20**, **22**, and **30**. In the following, we shall discuss only one from each pair because the other one will have exactly the same characteristics.

In Figure 2 we present in the second column for the 33 selected non-isoarithmic benzenoids **1**−**33** the number K of resonance formulas (traditionally also called Kekulé valence structures). In the fourth column one can see the π-electron partition for each of the eight benzenoid rings denoted by capital letters A−H. These partitions result as the row sum of entries in columns 5−11 divided by K. The sum of these eight partitions for each compound is the number of π electrons, totaling 30 π electrons. For each compound, the last line (boldface characters) lists in the fourth column the product hK that is also the row

TABLE 1: R_i and r_i Sequences (i = 0−6) of the 33 Non-isoarithmic Octaperifusenes with Four Contiguous Internal Vertices

no.	Clar	K	hK	R_6	R_5	R_4	R_3	R_2	R_1	R_0	r_6	r_5	r_4	r_3	r_2	r_1	r_0
1	2	18	144	4	29	50	49	12	0	0	0.222	1.611	2.778	2.722	0.667	0.000	0.000
2	2	19	152	10	22	52	56	12	0	0	0.526	1.158	2.737	2.947	0.632	0.000	0.000
3	3	22	176	6	39	56	55	20	0	0	0.273	1.773	2.545	2.500	0.909	0.000	0.000
4	3	23	184	16	30	51	66	21	0	0	0.696	1.304	2.217	2.870	0.913	0.000	0.000
5	3	24	192	14	35	53	69	21	0	0	0.583	1.458	2.208	2.875	0.875	0.000	0.000
6	3	25	200	18	32	56	70	24	0	0	0.720	1.280	2.240	2.800	0.960	0.000	0.000
7	3	26	208	16	37	57	75	23	0	0	0.615	1.423	2.192	2.885	0.885	0.000	0.000
8	3	26	208	19	45	58	51	23	10	2	0.731	1.731	2.231	1.962	0.885	0.385	0.077
9	3	26	208	6	57	66	46	25	7	1	0.231	2.192	2.538	1.769	0.962	0.269	0.038
10	3	27	216	21	48	58	52	22	12	3	0.778	1.778	2.148	1.926	0.815	0.444	0.111
11	3	28	224	9	67	67	43	20	14	4	0.321	2.393	2.393	1.536	0.714	0.500	0.143
12	3	29	232	19	51	67	57	26	10	2	0.655	1.759	2.310	1.966	0.897	0.345	0.069
13	3	29	232	18	49	69	58	30	7	1	0.621	1.690	2.379	2.000	1.034	0.241	0.034
14	3	30	240	8	75	68	45	29	12	3	0.267	2.500	2.267	1.500	0.967	0.400	0.100
15	3	30	240	25	55	59	56	29	13	3	0.833	1.833	1.967	1.867	0.967	0.433	0.100
16	3	31	248	20	57	70	58	30	11	2	0.645	1.839	2.258	1.871	0.968	0.355	0.065
17	3	31	248	27	58	58	58	29	14	4	0.871	1.871	1.871	1.871	0.935	0.452	0.129
18	3	32	256	21	71	64	46	34	17	3	0.656	2.219	2.000	1.438	1.063	0.531	0.094
19	3	32	256	9	93	68	28	31	23	4	0.281	2.906	2.125	0.875	0.969	0.719	0.125
20	4	34	272	20	71	67	64	37	11	2	0.588	2.088	1.971	1.882	1.088	0.324	0.059
21	4	35	280	26	71	67	63	33	16	4	0.743	2.029	1.914	1.800	0.943	0.457	0.114
22	4	36	288	22	77	69	67	36	14	3	0.611	2.139	1.917	1.861	1.000	0.389	0.083
23	4	36	288	27	85	65	44	39	23	5	0.750	2.361	1.806	1.222	1.083	0.639	0.139
24	4	36	288	11	111	69	30	33	27	7	0.306	3.083	1.917	0.833	0.917	0.750	0.194
25	4	36	288	34	86	60	36	34	30	8	0.944	2.389	1.667	1.000	0.944	0.833	0.222
26	4	37	296	29	87	67	44	38	25	6	0.784	2.351	1.811	1.189	1.027	0.676	0.162
27	4	37	296	23	92	62	54	41	20	4	0.622	2.486	1.676	1.459	1.108	0.541	0.108
28	4	37	296	29	91	60	46	39	25	6	0.784	2.459	1.622	1.243	1.054	0.676	0.162
29	4	38	304	29	93	64	47	39	26	6	0.763	2.447	1.684	1.237	1.026	0.684	0.158
30	4	39	312	25	98	68	50	42	24	5	0.641	2.513	1.744	1.282	1.077	0.615	0.128
31	4	39	312	31	99	60	47	40	28	7	0.795	2.538	1.538	1.205	1.026	0.718	0.179
32	4	40	320	32	116	50	32	49	34	7	0.800	2.900	1.250	0.800	1.225	0.850	0.175
33	5	45	360	40	138	52	22	50	46	12	0.889	3.067	1.156	0.489	1.111	1.022	0.267

sum of the boldface entries of the column sums for columns 5−11, which constitute the R_i sequence (with i = 6 through 0). The last column displays the structure of the benzenoid with capital letters for rings; when equivalent rings appear because of symmetry, they receive the same letter, as for **2**, **6**, **13**, **19**, **21**, **25**, **27**, and **33**.

Eric Clar expanded the information associated with Robinson's π-electron sextet circles,[32,33] in benzenoid formulas with such circles,[34] having observed that "sextet-resonant benzenoids" [35] (also called all-benzenoid aromatic hydrocarbons)[34] have a higher stability and lower tendency to react with dienophiles than isomeric benzenoids, which cannot accommodate such high numbers of sextet circles.[36] One can formulate accordingly the following three rules:[37−39] (i) no sextet circles are allowed in adjacent rings; (ii) all rings without a circle must have a Kekulé structure, that is, they need to have zero, one, or two double bonds and no sp^3-hybridized carbon atom; (iii) Clar structures must have maximum numbers of sextet circles subject to the above restrictions.

It must be mentioned that the known octaperifusenes with four internal vertices are shown in the book by Dias.[40] Trinajstić and co-workers[41] described the Wiswesser code for perifusenes that we used previously,[22] but this code is not presented in this communication.

In Figure 2 the partition of π electrons for rings having Clar sextets (which correspond to rings with high shares in the partition) are written in bold italics. The first two compounds in Figure 2 have only two Clar sextets; compounds **3**−**19** have three Clar sextets, compounds **20**−**32** have four Clar sextets, and compound **33** has five Clar sextets, being the unique sextet-resonant benzenoid (all-benzenoid compound) among the 33 non-isoarithmic octaperifusenes. Compound **6** has three pairs of equivalent rings, but only one of the two rings denoted by D can accommodate a Clar sextet;, therefore, only one D ring has the partition in bold italics.

The ordering of compounds **1**−**33** in Tables 1 and 2 is based on increasing K values, and for equal K the ordering is arbitrary. From the R_i sequence of Figure 2, which is repeated in Table 1, one obtains the r_i sequence by dividing each entry by the corresponding K value. Finally, from the r_i sequence one obtains the s_i sequence or *the benzenoid signature* shown in Table 2 by the definition $s_i = ir_i$.

There are seven numbers in the R_i and r_i sequences with i = 6 through 0, but only six in the s_i sequence with i = 6 through 1, because s_0 is always zero and is no longer included. For each compound, the sum $\Sigma_i r_i$ is the number 8 of rings, and the sum $\Sigma_i s_i$ is the number P = 30 of π electrons.

Conversion of Signatures into a Numerical Index for Characterizing Benzenoids

Although the signature, which is a sequence of six real numbers, could characterize a benzenoid, it is not a convenient instrument for this purpose. In order to convert it into a single number, we studied the correlation between numbers of Kekulé valence structures or Clar sextets and partial sums of s_i values, starting with singlets or quintets. One must note that there is a complementarity between such partial sums, so that all six indices must appear either in one or the other of the two partial sums, as indicated in Table 3; for brevity, the sum of doublets $s_i + s_j$ is denoted by s_{ij} (indices are in decreasing order), and so on for triplets, quartets, and quintets. The correlation Tables 4, 5, and 6 have the same absolute R^2 values for the two

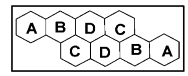
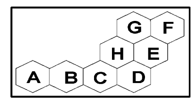
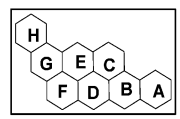
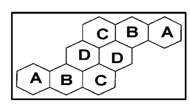
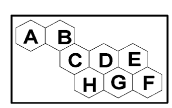
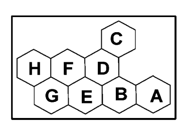
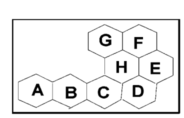
No.	*K*		Partition	*R6*	*R5*	*R4*	*R3*	*R2*	*R1*	*R0*	Structure
1	18	A	***4.67***	4	4	10	0	0	0	0	
		B	4.44	0	8	10	0	0	0	0	
		C	3.56	0	3	6	7	2	0	0	
		D	3.39	0	3	3	10	2	0	0	
		E	3.06	0	0	4	11	3	0	0	
		F	3.39	0	0	8	9	1	0	0	
		G	2.94	0	1	1	12	4	0	0	
		H	***4.56***	0	10	8	0	0	0	0	
			144	**4**	**29**	**50**	**49**	**12**	**0**	**0**	
2	19	2A	***4.79***	5	5	9	0	0	0	0	
		2B	3.84	0	4	9	5	1	0	0	
		2C	3.16	0	2	2	12	3	0	0	
		2D	3.21	0	0	6	11	2	0	0	
			152	**10**	**22**	**52**	**56**	**12**	**0**	**0**	
3	22	A	***4.82***	6	6	10	0	0	0	0	
		B	4.55	0	12	10	0	0	0	0	
		C	3.18	0	3	4	9	6	0	0	
		D	2.86	0	1	1	14	6	0	0	
		E	3.23	0	0	8	11	3	0	0	
		F	***4.64***	0	14	8	0	0	0	0	
		G	3.23	0	3	3	12	4	0	0	
		H	***3.50***	0	0	12	9	1	0	0	
			176	**6**	**39**	**56**	**55**	**20**	**0**	**0**	
4	23	A	***4.91***	7	7	9	0	0	0	0	
		B	3.74	0	5	9	7	2	0	0	
		C	3.39	0	4	4	12	3	0	0	
		D	3.09	0	0	6	13	4	0	0	
		E	***3.48***	0	0	12	10	1	0	0	
		F	2.87	0	1	1	15	6	0	0	
		G	3.35	0	4	5	9	5	0	0	
		H	***5.17***	9	9	5	0	0	0	0	
			184	**16**	**30**	**51**	**66**	**21**	**0**	**0**	
5	24	A	***5.25***	10	10	4	0	0	0	0	
		B	3.42	4	0	4	10	6	0	0	
		C	***3.96***	0	6	12	5	1	0	0	
		D	3.21	0	3	3	14	4	0	0	
		E	3.21	0	0	8	13	3	0	0	
		F	3.33	0	0	10	12	2	0	0	
		G	3.04	0	2	2	15	5	0	0	
		H	***4.58***	0	14	10	0	0	0	0	
			192	**14**	**35**	**53**	**69**	**21**	**0**	**0**	
6	25	2A	***5.08***	9	9	7	0	0	0	0	
		2B	3.52	0	5	7	9	4	0	0	
		2C	3.00	0	2	2	15	6	0	0	
		D	3.40	0	0	12	11	2	0	0	
		D	***3.40***	0	0	12	11	2	0	0	
			200	**18**	**32**	**56**	**70**	**24**	**0**	**0**	
7	25	A	***5.36***	10	10	6	0	0	0	0	
		B	3.92	6	0	6	10	4	0	0	
		C	***3.80***	0	6	8	9	3	0	0	
		D	3.52	0	0	12	12	2	0	0	
		E	3.28	0	3	3	15	5	0	0	
		F	***4.80***	0	16	10	0	0	0	0	
		G	3.40	0	0	10	13	3	0	0	
		H	3.12	0	2	2	16	6	0	0	
			208	**16**	**37**	**57**	**75**	**23**	**0**	**0**	
8	26	A	***4.81***	7	7	12	0	0	0	0	
		B	3.88	0	6	12	7	1	0	0	
		C	***5.38***	12	12	2	0	0	0	0	
		D	1.73	0	2	0	2	10	10	2	
		E	3.19	0	0	8	14	4	0	0	
		F	3.33	0	0	12	12	2	0	0	
		G	3.00	0	2	2	16	6	0	0	
		H	***4.62***	0	16	10	0	0	0	0	
			208	**19**	**45**	**58**	**51**	**23**	**10**	**2**	
9	26	A	***4.69***	6	6	14	0	0	0	0	
		B	4.46	0	12	14	0	0	0	0	
		C	3.62	0	5	8	11	2	0	0	
		D	3.12	0	3	3	14	6	0	0	
		E	***4.00***	0	8	11	6	1	0	0	
		F	3.42	0	5	5	12	4	0	0	
		G	***4.60***	0	18	8	0	0	0	0	
		H	2.00	0	0	3	3	12	7	1	
			208	**6**	**57**	**66**	**46**	**25**	**7**	**1**	

Figure 2. Part 1 of 4.

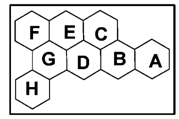
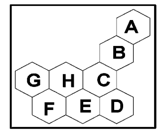
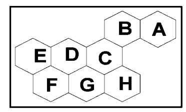
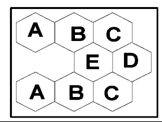
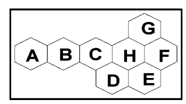
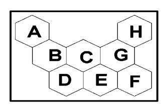
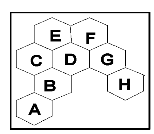
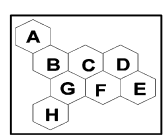
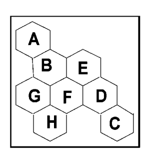
10	27	A	***4.89***	8	8	11	0	0	0	0	
		B	3.78	0	6	11	8	2	0	0	
		C	3.30	0	4	4	15	4	0	0	
		D	3.15	0	0	8	15	4	0	0	
		E	3.37	0	0	12	13	2	0	0	
		F	***4.59***	0	16	11	0	0	0	0	
		G	1.48	0	1	0	1	10	12	3	
		H	***5.44***	13	13	1	0	0	0	0	
			216	**21**	**48**	**58**	**52**	**22**	**12**	**3**	
11	28	A	***4.96***	9	9	10	0	0	0	0	
		B	4.64	0	18	10	0	0	0	0	
		C	1.36	0	1	0	1	8	14	4	
		D	***4.64***	0	18	10	0	0	0	0	
		E	3.36	0	0	13	12	3	0	0	
		F	3.11	0	3	3	16	6	0	0	
		G	***4.64***	0	18	10	0	0	0	0	
		H	3.32	0	0	12	13	3	0	0	
			224	**9**	**67**	**68**	**42**	**20**	**14**	**4**	
12	29	A	***5.03***	10	10	9	0	0	0	0	
		B	4.21	9	0	9	10	1	0	0	
		C	1.79	0	2	0	2	13	10	2	
		D	3.31	0	0	12	14	3	0	0	
		E	***4.62***	0	18	11	0	0	0	0	
		F	3.10	0	3	3	17	6	0	0	
		G	3.31	0	0	12	14	3	0	0	
		H	***4.62***	0	18	11	0	0	0	0	
			232	**19**	**51**	**67**	**57**	**26**	**10**	**2**	
13	29	2A	***4.93***	9	9	11	0	0	0	0	
		2B	3.79	0	7	11	9	2	0	0	
		2C	3.21	0	4	4	15	6	0	0	
		D	2.10	0	0	4	4	13	7	1	
		E	***4.03***	0	9	13	6	1	0	0	
			232	**18**	**49**	**69**	**58**	**30**	**7**	**1**	
14	30	A	***4.80***	8	8	14	0	0	0	0	
		B	4.53	0	16	14	0	0	0	0	
		C	3.33	0	5	6	13	6	0	0	
		D	3.80	0	9	9	9	3	0	0	
		E	***3.73***	0	8	9	10	3	0	0	
		F	3.57	0	7	7	12	4	0	0	
		G	***4.73***	0	22	8	0	0	0	0	
		H	1.47	0	0	1	1	12	13	3	
			240	**8**	**75**	**68**	**45**	**29**	**12**	**3**	
15	30	A	***5.10***	11	11	8	0	0	0	0	
		B	3.50	0	6	8	11	5	0	0	
		C	3.50	0	0	17	11	2	0	0	
		D	2.93	0	2	2	18	8	0	0	
		E	3.27	0	0	12	14	4	0	0	
		F	***4.67***	0	20	10	0	0	0	0	
		G	1.67	0	2	0	2	11	12	3	
		H	***5.40***	14	14	2	0	0	0	0	
			240	**25**	**55**	**59**	**56**	**29**	**13**	**3**	
16	31	A	***5.06***	11	11	9	0	0	0	0	
		B	3.61	0	7	9	11	4	0	0	
		C	3.68	0	8	8	12	3	0	0	
		D	1.71	0	0	2	2	14	11	2	
		E	***3.87***	0	9	11	9	2	0	0	
		F	3.29	0	5	5	15	6	0	0	
		G	3.90	0	8	13	9	1	0	0	
		H	***4.87***	9	9	13	0	0	0	0	
			248	**20**	**57**	**70**	**58**	**30**	**11**	**2**	
17	31	A	***5.16***	12	12	7	0	0	0	0	
		B	3.42	0	6	7	12	6	0	0	
		C	3.45	0	0	16	13	2	0	0	
		D	3.19	0	4	4	17	6	0	0	
		E	***4.65***	0	20	11	0	0	0	0	
		F	3.26	0	0	12	15	4	0	0	
		G	1.42	0	1	0	1	11	14	4	
		H	***5.45***	15	15	1	0	0	0	0	
			248	**27**	**58**	**58**	**58**	**29**	**14**	**4**	
18	32	A	***5.13***	12	12	8	0	0	0	0	
		B	2.63	0	6	2	6	11	6	1	
		C	***4.84***	9	9	14	0	0	0	0	
		D	3.91	0	8	14	9	1	0	0	
		E	3.44	0	6	6	16	4	0	0	
		F	1.72	0	0	2	2	15	11	2	
		G	3.66	0	8	8	13	3	0	0	
		H	***4.69***	0	22	10	0	0	0	0	
			256	**21**	**71**	**64**	**46**	**34**	**17**	**3**	

Figure 2. Part 2 of 4.

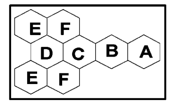
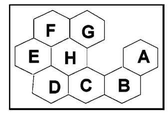
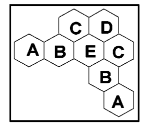
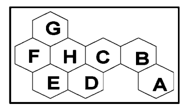
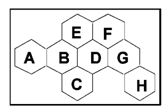
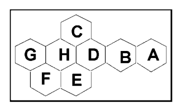
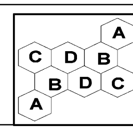
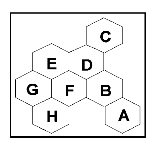
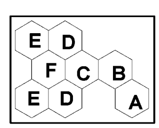
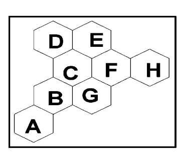
19	32	A	***4.84***	9	9	14	0	0	0	0	
		B	4.56	0	18	14	0	0	0	0	
		C	2.13	0	4	1	3	13	9	2	
		D	1.53	0	0	1	1	14	14	2	
		2E	***4.66***	0	10	8	12	2	0	0	
		2F	3.81	0	21	11	0	0	0	0	
			256	**9**	**93**	**68**	**28**	**31**	**23**	**4**	
20	34	A	***5.24***	14	14	6	0	0	0	0	
		B	3.47	6	0	6	14	8	0	0	
		C	***4.03***	0	10	16	7	1	0	0	
		D	3.35	0	6	6	16	6	0	0	
		E	***3.91***	0	10	13	9	2	0	0	
		F	3.47	0	7	7	15	5	0	0	
		G	***4.71***	0	24	10	0	0	0	0	
		H	1.82	0	0	3	3	15	11	2	
			272	**20**	**71**	**67**	**64**	**37**	**11**	**2**	
21	35	2A	***5.11***	13	13	9	0	0	0	0	
		2B	3.57	0	8	9	13	5	0	0	
		2C	***3.77***	0	10	10	12	3	0	0	
		D	3.69	0	9	10	12	4	0	0	
		E	1.40	0	0	1	1	13	16	4	
			280	**26**	**71**	**67**	**63**	**33**	**16**	**4**	
22	36	A	***5.17***	14	14	8	0	0	0	0	
		B	3.72	8	0	8	14	6	0	0	
		C	***3.81***	0	10	12	11	3	0	0	
		D	3.64	0	9	9	14	4	0	0	
		E	***3.81***	0	10	12	11	3	0	0	
		F	3.53	0	8	8	15	5	0	0	
		G	***4.72***	0	26	10	0	0	0	0	
		H	1.61	0	0	2	2	15	14	3	
			288	**22**	**77**	**69**	**67**	**36**	**14**	**3**	
23	36	A	***5.33***	16	16	4	0	0	0	0	
		B	1.94	0	4	0	4	13	12	3	
		C	***4.78***	0	28	8	0	0	0	0	
		D	1.92	0	0	4	4	15	11	2	
		E	***4.08***	0	12	16	7	1	0	0	
		F	3.19	0	5	5	18	8	0	0	
		G	3.83	0	9	14	11	2	0	0	
		H	***4.92***	11	11	14	0	0	0	0	
			288	**27**	**85**	**65**	**44**	**39**	**23**	**5**	
24	36	A	***4.92***	11	11	14	0	0	0	0	
		B	4.61	0	22	14	0	0	0	0	
		C	***4.83***	0	30	6	0	0	0	0	
		D	1.72	0	3	0	3	12	14	4	
		E	***4.06***	0	12	15	8	1	0	0	
		F	3.42	0	7	7	16	6	0	0	
		G	***4.72***	0	26	10	0	0	0	0	
		H	1.72	0	0	3	3	14	13	3	
			288	**11**	**111**	**69**	**30**	**33**	**27**	**7**	
25	36	2A	***5.42***	17	17	2	0	0	0	0	
		2B	1.58	0	2	0	2	13	15	4	
		2C	***4.67***	0	24	12	0	0	0	0	
		2D	3.33	0	0	16	16	4	0	0	
			288	**34**	**86**	**60**	**36**	**34**	**30**	**8**	
26	37	A	***4.97***	15	15	5	0	0	0	0	
		B	3.84	0	10	13	12	2	0	0	
		C	***5.38***	17	17	3	0	0	0	0	
		D	1.73	0	3	0	3	13	14	4	
		E	***4.05***	0	12	16	8	1	0	0	
		F	1.92	0	0	4	4	16	11	2	
		G	3.41	0	7	7	17	6	0	0	
		H	***4.70***	0	26	11	0	0	0	0	
			296	**29**	**87**	**67**	**44**	**38**	**25**	**6**	
27	37	A	***5.14***	14	14	9	0	0	0	0	
		B	3.84	9	0	9	14	5	0	0	
		C	***2.76***	0	8	2	8	12	6	1	
		2D	3.62	0	9	9	15	4	0	0	
		2E	***4.70***	0	26	11	0	0	0	0	
		F	1.35	0	0	2	2	16	4	3	
			296	**23**	**92**	**62**	**54**	**41**	**20**	**4**	
28	37	A	***5.14***	14	14	9	0	0	0	0	
		B	3.49	0	9	8	14	4	2	0	
		C	1.43	0	0	1	1	15	16	4	
		D	***4.70***	0	26	11	0	0	0	0	
		E	3.73	0	10	10	14	3	0	0	
		F	2.35	0	6	1	6	13	9	2	
		G	***3.92***	0	12	12	11	2	0	0	
		H	***5.22***	15	15	7	0	0	0	0	
			296	**29**	**92**	**59**	**46**	**37**	**27**	**6**	

Figure 2. Part 3 of 4.

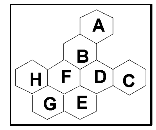
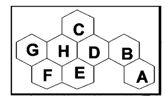
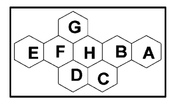
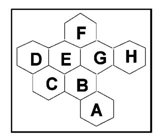
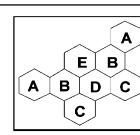
29	38	A	***5.03***	13	13	12	0	0	0	0	
		B	3.76	0	0	12	13	3	0	0	
		C	***5.26***	16	16	6	0	0	0	0	
		D	2.26	0	6	0	6	14	10	2	
		E	***3.95***	0	12	14	10	2	0	0	
		F	1.53	0	0	2	2	14	16	4	
		G	3.47	0	8	8	16	6	0	0	
		H	***4.74***	0	28	10	0	0	0	0	
			304	**29**	**93**	**64**	**47**	**39**	**26**	**6**	
30	39	A	***5.08***	14	14	11	0	0	0	0	
		B	4.05	11	0	11	14	3	0	0	
		C	***4.77***	0	30	9	0	0	0	0	
		D	2.26	0	6	0	6	15	10	2	
		E	***3.95***	0	12	15	10	2	0	0	
		F	3.46	0	8	8	17	6	0	0	
		G	***4.72***	0	28	11	0	0	0	0	
		H	1.72	0	0	3	3	16	14	3	
			312	**25**	**98**	**68**	**50**	**42**	**24**	**5**	
31	39	A	***5.08***	14	14	11	0	0	0	0	
		B	3.62	0	9	11	14	5	0	0	
		C	3.67	0	10	10	15	4	0	0	
		D	***3.92***	0	12	14	11	2	0	0	
		E	***5.31***	17	17	5	0	0	0	0	
		F	2.05	0	5	0	5	14	12	3	
		G	***4.82***	0	32	7	0	0	0	0	
		H	1.54	0	0	2	2	15	16	4	
			312	**31**	**99**	**60**	**47**	**40**	**28**	**7**	
32	40	A	***5.13***	15	15	10	0	0	0	0	
		B	2.68	0	8	2	8	14	7	1	
		C	3.65	0	10	10	16	4	0	0	
		D	***4.70***	0	28	12	0	0	0	0	
		E	1.55	0	0	2	2	26	16	4	
		F	***4.80***	0	32	8	0	0	0	0	
		G	2.23	0	6	0	6	15	12	1	
		H	***5.28***	17	17	6	0	0	0	0	
			320	**32**	**116**	**50**	**32**	**49**	**35**	**6**	
33	45	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	
			360	**40**	**138**	**52**	**22**	**50**	**46**	**12**	

Figure 2. Thirty-three non-isoarithmic octaperifusenes having four contiguous internal vertices with their partition and R_i sequences.

complementary multiplets but they are either positive or negative. In the following we shall adopt for each complementary pair the multiplet with positive R^2 values.

In all three Tables 4, 5, and 6, one sees the same satisfactory value (Pearson product-moment correlation coefficient $R = 0.925$) for the intercorrelation between numbers of Kekulé valence structures and Clar sextets; therefore, in the following discussion we will concentrate only on correlations between partial signature sums and K values.

Starting with singlet/quintet sum correlations with the number K of Kekulé valence structures, one sees from Table 4 that s_4 has the largest negative R value; therefore s_{65321} will have the same largest positive $R = 0.922$ value. Then from Table 5 one sees that s_{43} has the largest negative R value (corresponding to s_{6521} with the same largest positive $R = 0.953$), followed by s_{21} and s_{65} with positive R values. Finally, from Table 6 one sees that the largest R value is for s_{134} (corresponding to the same largest positive s_{652} with $R = 0.957$) followed by $s_{651.}$

Also indicated in Table 3 for each compound are partial signature sums $s_6 + s_5 + s_2 + s_1$ (denoted for brevity by s_{6521}), $s_6 + s_5$ (denoted as s_{65}), and $s_2 + s_1$ (denoted as s_{21}). We do not include $s_4 + s_3$ (denoted as s_{43}) because this doublet sum is complementary to the quadruplet sum s_{6521}. One can observe that although on going from **1** to **33** s_{21} increases about twice and has small values the other sums have larger values; s_{6521} and s_{65} also increases about twice. Most interestingly, in a plot of s_{65} versus s_{6521} there is an almost perfect linear correlation with the coefficient of determination $R^2 = 0.998$, as seen in Figure 3.

These observations can be explained by the fact that s_1 is quite small relative to the other terms of the signature (for benzenoids **1**−**7** it is actually zero) and that, as seen from Table 4, K is negatively correlated with s_4 and s_3 but positively correlated with all four remaining terms. From the following tables, one sees that K is fairly well correlated with $s_6 + s_5 + s_2$ (denoted by s_{652}) and $s_6 + s_5 + s_2 + s_1$ (denoted by s_{6521}) with $R^2 = 0.957$ and 0.953, respectively; therefore, these two partial sums have been included in Table 3.

An interesting correlation is found between the number K of resonance structures and the sums $s_6 + s_5 + s_2$ or $s_6 + s_5 + s_2 + s_1$ (coefficients of determination $R^2 = 0.915$ and 0.909, respectively), as seen in Figure 4; there is an almost perfect agreement between these two plots, although as will be seen in the next section, there are small differences in the ordering of benzenoids between s_{652} and s_{6521}. A slightly lower correlation for K exists with the sum $s_6 + s_5$ ($R^2 = 0.899$), as one could expect because s_{6521} and s_{65} are strongly intercorrelated.

There is an explanation about these correlations, namely in the way the 30 π electrons of the 33 octaperifusenes analyzed in the present paper are distributed. For the compounds at the end of the list, which have 4 or 5 Clar sextets, the sum $s_6 + s_5$ is large and $s_4 + s_3$ is small, whereas for the compounds at

TABLE 2: Signatures (s_i Sequences with $i = 1-6$) and Signature Partial Sums for Octaperifusenes with Four Contiguous Internal Vertices Ordered According to Increasing K Values

no.	Clar	K	s_6	s_5	s_4	s_3	s_2	s_1	s_{652}	s_{6521}	s_{65}	s_{21}
1	2	18	1.333	8.056	11.111	8.167	1.333	0.000	10.722	10.722	9.389	1.333
2	2	19	3.158	5.789	10.947	8.842	1.263	0.000	10.210	10.210	8.947	1.263
3	3	22	1.636	8.864	10.182	7.500	1.818	0.000	12.318	12.318	10.500	1.818
4	3	23	4.174	6.522	8.870	8.609	1.826	0.000	12.522	12.522	10.696	1.826
5	3	24	3.500	7.292	8.833	8.625	1.750	0.000	12.542	12.542	10.792	1.750
6	3	25	4.320	6.400	8.960	8.400	1.920	0.000	12.640	12.640	10.720	1.920
7	3	26	3.692	7.115	8.769	8.654	1.769	0.000	12.576	12.576	10.807	1.769
9	3	26	1.385	10.962	10.154	5.308	1.923	0.269	14.270	14.539	12.347	2.192
8	3	26	4.385	8.654	8.923	5.885	1.769	0.385	14.808	15.193	13.039	2.154
10	3	27	4.667	8.889	8.593	5.778	1.630	0.444	15.186	15.630	13.556	2.074
11	3	28	1.929	11.964	9.571	4.607	1.429	0.500	15.322	15.822	13.893	1.929
13	3	29	3.724	8.448	9.517	6.000	2.069	0.241	14.241	14.482	12.172	2.310
12	3	29	3.931	8.793	9.241	5.897	1.793	0.345	14.517	14.862	12.724	2.138
14	3	30	1.600	12.500	9.067	4.500	1.933	0.400	16.033	16.433	14.100	2.333
15	3	30	5.000	9.167	7.867	5.600	1.933	0.433	16.100	16.533	14.167	2.366
16	3	31	3.871	9.194	9.032	5.613	1.935	0.355	15.000	15.355	13.065	2.290
17	3	31	5.226	9.355	7.484	5.613	1.871	0.452	16.452	16.904	14.581	2.323
18	3	32	3.938	11.094	8.000	4.313	2.125	0.531	17.157	17.688	15.032	2.656
19	3	32	1.688	14.531	8.500	2.625	1.938	0.719	18.157	18.876	16.219	2.657
20	4	34	3.529	10.441	7.882	5.647	2.176	0.324	16.146	16.470	13.970	2.500
21	4	35	4.457	10.143	7.657	5.400	1.886	0.457	16.486	16.943	14.600	2.343
22	4	36	3.667	10.694	7.667	5.583	2.000	0.389	16.361	16.750	14.361	2.389
23	4	36	4.500	11.806	7.222	3.667	2.167	0.639	18.473	19.112	16.306	2.806
24	4	36	1.833	15.417	7.667	2.500	1.833	0.750	19.083	19.833	17.250	2.583
25	4	36	5.667	11.944	6.667	3.000	1.889	0.833	19.500	20.333	17.611	2.722
27	4	37	3.730	12.432	6.703	4.378	2.216	0.541	18.378	18.919	16.162	2.757
26	4	37	4.703	11.757	7.243	3.568	2.054	0.676	18.514	19.190	16.460	2.730
28	4	37	4.703	12.297	6.486	3.730	2.108	0.676	19.108	19.784	17.000	2.784
29	4	38	4.579	12.237	6.737	3.711	2.053	0.684	18.869	19.553	16.816	2.737
30	4	39	3.846	12.564	6.974	3.846	2.154	0.615	18.564	19.179	16.410	2.769
31	4	39	4.769	12.692	6.154	3.615	2.051	0.718	19.512	20.230	17.461	2.769
32	4	40	4.800	14.500	5.000	2.400	2.450	0.850	21.750	22.600	19.300	3.300
33	5	45	5.333	15.333	4.622	1.467	2.222	1.022	22.888	23.910	20.666	3.244

TABLE 3: Complementary Signature Partial Sums (on Top of Each Other)

Complementary singlets/quintets:

s_6	s_5	s_4	s_3	s_2	s_1
s_{54321}	s_{64321}	s_{65321}	s_{65421}	s_{65431}	s_{65432}

Complementary doublets/quartets:

s_{21}	s_{31}	s_{41}	s_{51}	s_{61}	s_{32}	s_{42}	s_{52}	s_{62}	s_{43}	s_{53}	s_{63}	s_{54}	s_{64}	s_{65}
s_{6543}	s_{6542}	s_{6532}	s_{6432}	s_{5432}	s_{6541}	s_{6531}	s_{6431}	s_{5431}	s_{6521}	s_{6421}	s_{5421}	s_{6321}	s_{5321}	s_{4321}

Complementary triplets/triplets:

s_{321}	s_{421}	s_{521}	s_{621}	s_{431}	s_{531}	s_{631}	s_{541}	s_{641}	s_{651}
s_{654}	s_{653}	s_{643}	s_{543}	s_{652}	s_{642}	s_{542}	s_{632}	s_{532}	s_{432}

TABLE 4: Correlation between s_i and the Numbers of Clar or Kekulé Structures

	Clar	K	s_6	s_5	s_4	s_3	s_2	s_1
Clar	1.000							
K	0.925	1.000						
s_6	0.472	0.485	1.000					
s_5	0.710	0.815	−0.008	1.000				
s_4	−0.887	−0.922	−0.663	−0.685	1.000			
s_3	−0.728	−0.867	−0.212	−0.952	0.740	1.000		
s_2	0.746	0.786	0.425	0.568	−0.772	−0.611	1.000	
s_1	0.758	0.892	0.383	0.897	−0.820	−0.976	0.580	1.000

the beginning of the list with 2 or 3 Clar sextets the reverse is true. All 33 octaperifusenes appear ordered in Table 3 according to increasing numbers of Clar sextets, from 2 to 5 (these numbers are indicated in the column headed as ‘Clar’ in Tables 4, 5, and 6). Such linear correlations between sums $s_6 + s_5$ and $s_4 + s_3$ are general and they depend on the number of rings, on branching, and for perifusenes on the number of internal vertices.

In a recent paper,[42] a transition by means of Clar, Fries, quasi-Clar, anti-Fries, and Kekulé valence structures was proposed between the two different ways of keeping account of the π electrons among rings of benzenoids, namely either via partitions (i.e., row sums in arrays such as those presented in Figure 2) or via signatures (i.e., column sums in these arrays).

Ordering of Benzenoids

The two parameters s_{256} and s_{1256} can serve not only for characterizing benzenoids, but also for providing an ordering

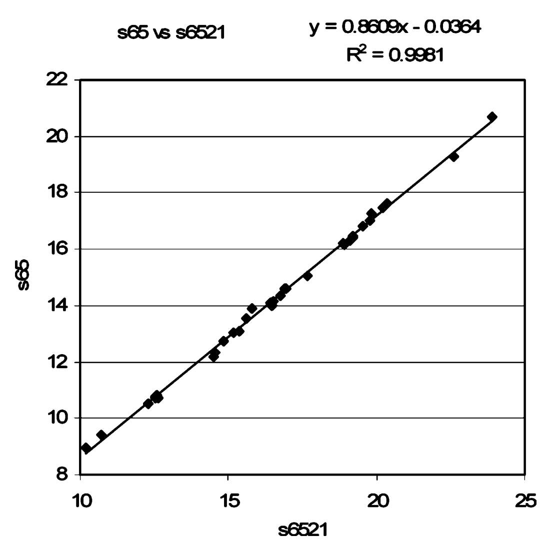


Figure 3. Plot of the sum $s_6 + s_5$ versus the sum $s_6 + s_5 + s_2 + s_1$.

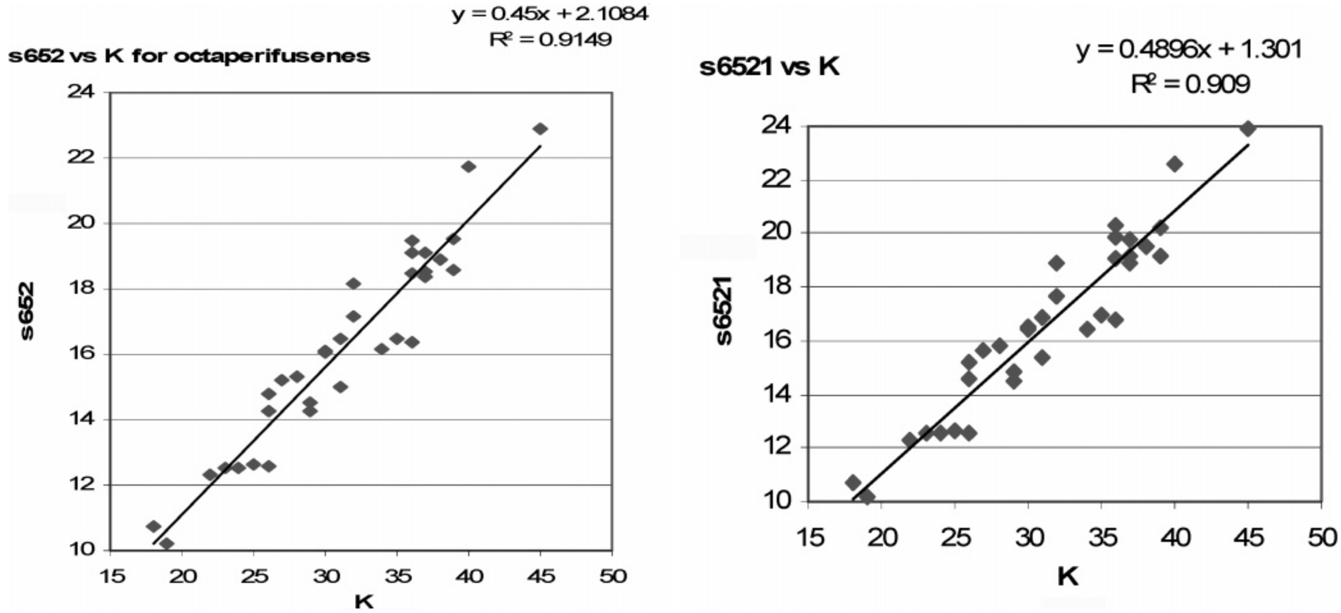


Figure 4. Plots of coefficients of determination of s_{652} and s_{6521} versus the number K of Kekulé structures for the 33 selected octaperifusenes.

TABLE 5: Correlation between Signature Pair Sums ($s_i + s_j$) and Numbers of Clar or Kekulé Structures

	Clar	K	s_1+s_2	s_1+s_3	s_1+s_4	s_1+s_5	s_1+s_6	s_2+s_3	s_2+s_4	s_2+s_5	s_2+s_6	s_3+s_4	s_3+s_5	s_3+s_6	s_4+s_5	s_4+s_6	s_5+s_6
Clar	1.000																
K	0.925	1.000															
s_1+s_2	0.846	0.947	1.000														
s_1+s_3	−0.720	−0.859	−0.902	1.000													
s_1+s_4	−0.873	−0.885	−0.852	0.636	1.000												
s_1+s_5	0.722	0.830	0.851	−0.966	−0.624	1.000											
s_1+s_6	0.583	0.623	0.596	−0.366	−0.779	0.218	1.000										
s_2+s_3	−0.684	−0.828	−0.858	0.993	0.599	−0.959	−0.357	1.000									
s_2+s_4	−0.869	−0.902	−0.856	0.709	0.983	−0.694	−0.780	0.691	1.000								
s_2+s_5	0.740	0.842	0.870	−0.960	−0.643	0.997	0.215	−0.944	−0.699	1.000							
s_2+s_6	0.565	0.585	0.571	−0.279	−0.772	0.133	0.984	−0.252	−0.740	0.143	1.000						
s_3+s_4	−0.852	−0.953	−0.965	0.943	0.854	−0.912	−0.593	0.927	0.900	−0.914	−0.527	1.000					
s_3+s_5	0.395	0.383	0.357	−0.490	−0.263	0.694	−0.375	−0.478	−0.288	0.706	−0.409	−0.426	1.000				
s_3+s_6	−0.416	−0.539	−0.595	0.840	0.216	−0.894	0.197	0.842	0.297	−0.886	0.284	0.649	−0.741	1.000			
s_4+s_5	0.256	0.370	0.420	−0.721	−0.029	0.795	−0.372	−0.734	−0.120	0.782	−0.464	−0.490	0.747	−0.979	1.000		
s_4+s_6	−0.655	−0.687	−0.689	0.751	0.555	−0.889	0.046	0.724	0.576	−0.906	0.083	0.728	−0.923	0.820	−0.752	1.000	
s_5+s_6	0.847	0.948	0.953	−0.944	−0.849	0.916	0.589	−0.932	−0.902	0.915	0.517	−0.999	0.435	−0.654	0.498	−0.729	1.000

TABLE 6: Correlation between Signature Triplet Sums (s_{ijk}) and Numbers of Clar or Kekulé Structures

	Clar	K	s_{123}	s_{124}	s_{125}	s_{126}	s_{134}	s_{135}	s_{136}	s_{145}	s_{146}	s_{156}
Clar	1											
K	0.925	1										
s_{123}	−0.667	−0.812	1									
s_{124}	−0.849	−0.854	0.549	1								
s_{125}	0.748	0.854	−0.956	−0.625	1							
s_{126}	0.652	0.695	−0.374	−0.833	0.330	1						
s_{134}	−0.859	−0.957	0.906	0.838	−0.925	−0.662	1					
s_{135}	0.549	0.576	−0.690	−0.417	0.84	−0.094	−0.637	1				
s_{136}	−0.345	−0.461	0.805	0.086	−0.827	0.223	0.563	−0.827	1			
s_{145}	0.339	0.462	−0.829	−0.100	0.830	−0.203	−0.574	0.815	−0.994	1		
s_{146}	−0.546	−0.545	0.576	0.398	−0.775	0.113	0.576	−0.971	0.758	−0.722	1	
s_{156}	0.841	0.945	−0.924	−0.824	0.929	0.646	−0.997	0.641	−0.579	0.598	−0.563	1

criterion for isomeric benzenoids, that is, benzenoids with the same h and a values. In Table 7 one can see the ordering of the 33 selected octaperifusenes according to the above two parameters; they differ only in four inversions between neighboring pairs of benzenoids: **15**/**20**, **30**/**26**, **24**/**28**, and **25**/**31**. As a result, although the ordering by these two parameters is rather similar, it differs appreciably from the initial ordering resulting in the sequential values **1**−**33**. However, the lower (2) and higher values (5) of Clar sextets are the same for all three orderings (Tables 2, 7, and 8) and there are only a few cases for benzenoids with 3 and 4 Clar sextets that are mixed up at the middle of Tables 7 and 8.

For catafusenes, better results than those with the above two parameters are obtained with s_{126}, but for the correlation with K of the 33 perifusenes analyzed in this paper, the coefficient of determination is low, $R^2 = 0.483$.

TABLE 7: Signatures of the 33 Non-isoarithmic Octaperifusenes Sorted by Increasing s_{6521}

no.	Clar	K	hK	s_6	s_5	s_4	s_3	s_2	s_1	s_{6521}
2	2	19	152	3.158	5.789	10.947	8.842	1.263	0.000	10.211
1	2	18	144	1.333	8.056	11.111	8.167	1.333	0.000	10.722
3	3	22	176	1.636	8.864	10.182	7.500	1.818	0.000	12.318
4	3	23	184	4.174	6.522	8.870	8.609	1.826	0.000	12.522
5	3	24	192	3.500	7.292	8.833	8.625	1.750	0.000	12.542
7	3	26	208	3.692	7.115	8.769	8.654	1.769	0.000	12.577
6	3	25	200	4.320	6.400	8.960	8.400	1.920	0.000	12.640
13	3	29	232	3.724	8.448	9.517	6.000	2.069	0.241	14.483
9	3	26	208	1.385	10.962	10.154	5.308	1.923	0.269	14.538
12	3	29	232	3.931	8.793	9.241	5.897	1.793	0.345	14.862
8	3	26	208	4.385	8.654	8.923	5.885	1.769	0.385	15.192
16	3	31	248	3.871	9.194	9.032	5.613	1.935	0.355	15.355
10	3	27	216	4.667	8.889	8.593	5.778	1.630	0.444	15.630
11	3	28	224	1.929	11.964	9.571	4.607	1.429	0.500	15.821
14	3	30	240	1.600	12.500	9.067	4.500	1.933	0.400	16.433
20	4	34	272	3.529	10.441	7.882	5.647	2.176	0.324	16.471
15	3	30	240	5.000	9.167	7.867	5.600	1.933	0.433	16.533
22	4	36	288	3.667	10.694	7.667	5.583	2.000	0.389	16.750
17	3	31	248	5.226	9.355	7.484	5.613	1.871	0.452	16.903
21	4	35	280	4.457	10.143	7.657	5.400	1.886	0.457	16.943
18	3	32	256	3.938	11.094	8.000	4.313	2.125	0.531	17.688
19	3	32	256	1.688	14.531	8.500	2.625	1.938	0.719	18.875
27	4	37	296	3.730	12.432	6.703	4.378	2.216	0.541	18.919
23	4	36	288	4.500	11.806	7.222	3.667	2.167	0.639	19.111
30	4	39	312	3.846	12.564	6.974	3.846	2.154	0.615	19.179
26	4	37	296	4.703	11.757	7.243	3.568	2.054	0.676	19.189
29	4	38	304	4.579	12.237	6.737	3.711	2.053	0.684	19.553
28	4	37	296	4.703	12.297	6.486	3.730	2.108	0.676	19.784
24	4	36	288	1.833	15.417	7.667	2.500	1.833	0.750	19.833
31	4	39	312	4.769	12.692	6.154	3.615	2.051	0.718	20.231
25	4	36	288	5.667	11.944	6.667	3.000	1.889	0.833	20.333
32	4	40	320	4.800	14.500	5.000	2.400	2.450	0.850	22.600
33	5	45	360	5.333	15.333	4.622	1.467	2.222	1.022	23.911

TABLE 8: Signatures of the 33 Non-isoarithmic Octaperifusenes Sorted by Increasing s_{652}

no.	Clar	K	hK	s_6	s_5	s_4	s_3	s_2	s_1	s_{652}
2	2	19	152	3.158	5.789	10.947	8.842	1.263	0.000	10.210
1	2	18	144	1.333	8.056	11.111	8.167	1.333	0.000	10.722
3	3	22	176	1.636	8.864	10.182	7.500	1.818	0.000	12.318
4	3	23	184	4.174	6.522	8.870	8.609	1.826	0.000	12.522
5	3	24	192	3.500	7.292	8.833	8.625	1.750	0.000	12.542
7	3	26	208	3.692	7.115	8.769	8.654	1.769	0.000	12.576
6	3	25	200	4.320	6.400	8.960	8.400	1.920	0.000	12.640
13	3	29	232	3.724	8.448	9.517	6.000	2.069	0.241	14.241
9	3	26	208	1.385	10.962	10.154	5.308	1.923	0.269	14.270
12	3	29	232	3.931	8.793	9.241	5.897	1.793	0.345	14.517
8	3	26	208	4.385	8.654	8.923	5.885	1.769	0.385	14.808
16	3	31	248	3.871	9.194	9.032	5.613	1.935	0.355	15.000
10	3	27	216	4.667	8.889	8.593	5.778	1.630	0.444	15.186
11	3	28	224	1.929	11.964	9.571	4.607	1.429	0.500	15.322
14	3	30	240	1.600	12.500	9.067	4.500	1.933	0.400	16.033
15	3	30	240	5.000	9.167	7.867	5.600	1.933	0.433	16.100
20	4	34	272	3.529	10.441	7.882	5.647	2.176	0.324	16.146
22	4	36	288	3.667	10.694	7.667	5.583	2.000	0.389	16.361
17	3	31	248	5.226	9.355	7.484	5.613	1.871	0.452	16.452
21	4	35	280	4.457	10.143	7.657	5.400	1.886	0.457	16.486
18	3	32	256	3.938	11.094	8.000	4.313	2.125	0.531	17.157
19	4	32	256	1.688	14.531	8.500	2.625	1.938	0.719	18.157
27	4	37	296	3.730	12.432	6.703	4.378	2.216	0.541	18.378
23	4	36	288	4.500	11.806	7.222	3.667	2.167	0.639	18.473
26	4	37	296	4.703	11.757	7.243	3.568	2.054	0.676	18.514
30	4	39	312	3.846	12.564	6.974	3.846	2.154	0.615	18.564
29	4	38	304	4.579	12.237	6.737	3.711	2.053	0.684	18.869
24	4	36	288	1.833	15.417	7.667	2.500	1.833	0.750	19.083
28	4	37	296	4.703	12.297	6.486	3.730	2.108	0.676	19.108
25	4	36	288	5.667	11.944	6.667	3.000	1.889	0.833	19.500
31	4	39	312	4.769	12.692	6.154	3.615	2.051	0.718	19.512
32	4	40	320	4.800	14.500	5.000	2.400	2.450	0.850	21.750
33	5	45	360	5.333	15.333	4.622	1.467	2.222	1.022	22.888

Conclusions

By selecting a representative set of *peri*-condensed benzenoids, namely 33 non-isoarithmic octaperifusenes, and compressing the recently devised benzenoid signature with six real numbers into a single partial sum, it was shown that two partial sums (s_{256} followed closely by s_{1256}) can characterize benzenoids and can serve as ordering criteria.

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