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Perfect Matchings in Polyhexes, or Recent Graph-theoretical Contributions to Benzenoids[1]

Alexandru T. Balaban
(Texas A&M University at Galveston, 5007 Avenue U, Galveston, TX, USA
Email: `balabana@tamug.edu`)

Milan Randić
(National Institute of Chemistry, Hajdrikova 19, SI-1000 Ljubljana, Slovenia;
Department of Math. & Comp. Sci., Drake University, Des Moines, Iowa, USA
Email: `mrandic@msn.com`)

Abstract: After an introduction on the history of polycyclic aromatic compounds, recent advances in the theory of benzenoids are briefly reviewed. Then using systems with 4, 5, or 6 benzenoid rings for illustration, the partition of the P π-electrons among the rings of the benzenoid is presented, followed by a different way of examining the distribution of these π-electrons which is called the signature of the benzenoid, consisting in six integers from s_6 to s_1. The P π-electrons are divided between the two sums $s_6 + s_5 + s_2 + s_1$ and $s_4 + s_3$ characterizing thereby the closeness of benzenoids to all-resonant structures according to Clars theory.

Key Words: Perfect matchings (1-factors, resonance structures, or Kekulé structures); polycyclic aromatic hydrocarbons (polyhexes or benzenoids); isoarithmic benzenoids; Clar structures.

Category: G.2.2, J.2

1 Introduction: Aromatic compounds, benzenoids, and perfect matchings (Kekulé structures)

In order to understand better the importance of this topic for chemistry, a historical preamble is needed. In the second half of the 19th century chemistry blossomed from an empirical-technological trade to a real science. A brief time before the end of the 18th century, in England, Dalton advanced his atomic theory, Priestley discovered oxygen, Davy discovered how to isolate alkaline metals by electrolysis of their molten chlorides, and Faraday formulated the laws of electrochemistry; and in France, Lavoisier introduced scientific terms and notation for chemical elements, substances, and reactions. By showing that the phlogiston theory had no scientific basis, Lavoisier removed one of the dogmas inherited from the dark ages of alchemy, but with his execution by guillotine during the French Revolution, France lost much of its impact in chemistry. Contributions

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[1] C. S. Calude, G. Stefanescu, and M. Zimand (eds.). *Combinatorics and Related Areas. A Collection of Papers in Honour of the 65th Birthday of Ioan Tomescu.*

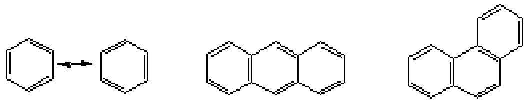
from Sweden (with Berzelius and Scheele) were important, but the greatest advances were made by German chemists. We will start by mentioning Whler, who was responsible for removing another dogma about the vital force, which was believed to be the only way for making organic substances, and Liebig, who put forward the method for determining by chemical analysis the constitutional formulas of organic compounds, and who discovered that fertilizers could improve substantially the yield of agricultural crops. Later, at the beginning of the 20th century it was again thanks to discoveries by German chemists (Ostwald, Haber, and Bosch) that nitrogen fertilizers could be made from air and water.

It was around 1850 that most organic compounds were shown to react predictably according to the ratio between the numbers of hydrogen and carbon atoms, which could attain a maximum value for a certain composition. For acyclic hydrocarbons, such a maximum value corresponded to formula C_nH_{2n+2} and these saturated alkanes could react only by substituting some of the hydrogens by other atoms such as halogens or oxygen. At lower C/H ratios, analogous acyclic hydrocarbons behaved differently, namely by adding hydrogens (or halogens) to attain the maximum ratio, and were termed unsaturated. Chemists were puzzled, however, by a group of substances that behaved puzzlingly: although they were hydrogen-poor, they did not react by addition but rather by substitution. In the absence of a class name based on chemical structure, at that time chemists designated them by the term aromatic because most of the known representatives at that time (e. g. benzene C_6H_6 –discovered by Faraday around 1820–, toluene, or benzaldehyde) had distinct aromas. Nowadays this term aromatic compounds continues to be used but it denotes just those compounds containing a certain type of chemical bonding without any connection to smell.

Kekulé was responsible for solving around 1860 this problem. He had already proved that carbon atoms are tetravalent, and he argued that unsaturated organic compounds possessed double or triple carbon-carbon bonds that could become saturated by adding two or four hydrogen atoms, respectively. However, when alternating single and double bonds (called conjugated double bonds) occurred in a cyclic compound, the effect was a special type of bonding (present in benzene, the prototype of aromatic compounds), resulting in the tendency to react readily by substitution rather than by addition, which occurred only under harsh conditions. In 1860, Kekulé organized in Karlsruhe the first international chemical congress, where Cannizzaros lecture about Avogadros previously advocated and forgotten ideas helped to elucidate the difference between atoms and molecules as the smallest particles of matter. As a consequence, the atomic weights of elements could be put on a true basis, and this helped Mendeleev to elaborate his Periodic System of elements. During the two decades preceding the 2nd World War a convergent evolution of quantum theories in physics and chemistry put Kekulés ides on firm scientific ground, thanks to Linus Pauling in

USA, Robert Robinson in England, and Erich Hckel in Germany. The delocalized sextet of π-electrons in the two possible Kekulé structures of benzene (1) are said to be resonant and contribute equally to describing the true distribution of these electrons in the molecule. Now chemists were on the right track to understand molecular structure, to predict all possible isomers (substances with a given molecular formula but with different structures and properties, originating in various ways of connecting atoms). In turn, this allowed chemists to develop new medicines, dyestuffs, fertilizers, detergents, plastics, textile fibers, elastomers, construction materials, etc.

Benzenoid hydrocarbons (benzenoids, for short) have fused (condensed) six-membered rings when two rings share one CC bond. The simplest pair of isomeric benzenoids share the molecular formula $C_{14}H_{10}$ involving three condensed rings and are called anthracene (2) with linearly-used rings, and phenanthrene with angularly-fused rings or kinked fusion (3).



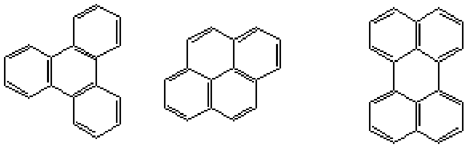
1 2 3

Figure 1: Benzene (1), anthracene (2), and phenanthrene (3)

An intermezzo about organic chemical formulas: hydrogen atoms are usually omitted for simplicity, as they are easy to place such that carbon atoms are always tetravalent (or in graph-theoretical terms, whenever a graph vertex symbolizing a carbon atom has vertex degrees lower than four). A line (graph edge) symbolizes a pair of shared electrons between two atoms. Kekulés pair of benzene formulas indicate that there are two possibilities for this sharing so that the three double bonds (six π-electrons) are delocalized over the whole ring, making this π-electron sextet reluctant to addition and prone to substitution reactions that conserve this sextet. Non-aromatic substances have double bonds that are shorter (1.33 Å) than single bonds (1.54 Å), but benzene has six equally long bonds (1.40 Å). This electronic delocalization stabilizes aromatic substances, making them resistant to heat or oxidizers that destroy non-aromatic substances.

From the approximately 30 million known substances recorded till now in the Chemical Abstracts databank, about half have aromatic rings (although hydrocarbons are only a minority among them). All constituents of genes (DNA, RNA) contain heterocyclic aromatic systems, and some of the amino acids essential to proteins and life have aromatic rings. The most stable plastics are those with aromatic systems. To understand the chemistry of organic compounds, chemists consider them as being derived from the simplest organic substances, namely hydrocarbons (composed only of C and H atoms); hydrogens may be substituted by other atoms or groups, and carbon atoms may be replaced by other atoms (named heteroatoms) such as nitrogen. The importance of polycyclic aromatic hydrocarbons is also connected with the fact that some benzenoids such as benzopyrene (present in tobacco smoke and in exhaust gases) are carcinogenic.

A carbon atom in a polycyclic aromatic hydrocarbon may be connected to two carbon atoms and a hydrogen atom, or to three carbon atoms. A C–H group must be a part of a single ring, but a carbon atom with no attached hydrogen may belong either to two rings (called cata-condensed or cata-fused rings) or to three rings (called peri-condensed or peri-fused rings). Benzene (1), anthracene (2), phenanthrene (3) and triphenylene (4) are all examples of catafusenes, whereas pyrene (5) or perylene (6) exemplify perifusenes.



4 5 6

Figure 2: Triphenylene (4), pyrene (5), and perylene (6)

Another way of viewing cata/peri-condensation of benzenoids involves the inner dual of graphs formed by vertices at the centers of hexagons and by edges connecting vertices corresponding to rings sharing a CC bond: catafusenes have acyclic inner duals (dualists) whereas perifusenes have dualists with triangles.

Chemists had found that phenanthrene (3) was more stable than its isomer anthracene (2). Pauling correlated this difference with the fact that there exist five Kekulé structures (also called resonance structures) of phenanthrene, while there are only four for anthracene. In graph theory, Kekulé structures are equivalent to perfect matchings or to 1-factors of the corresponding graphs. From the ratio between the number of Kekulé structures in which a particular CC bond was double and the total number of all Kekulé structures, Pauling derived the bond order that correlated well with experimentally determined bond lengths in benzenoids.

For more than 45 years, the present authors have been interested in chemical applications of graph theory and in aromaticity. The first author had published in 1959 an article in Romanian language involving both these topics [Balaban 1959]. On the advice of his childhood friend, Silviu Teleman, he contacted Frank Harary, with whom he later collaborated in ten joint publications. Among mathematicians from Romania, he collaborated with Professors Solomon Marcus and Ioan Tomescu. Joint publications with the latter mathematician [Balaban and Tomescu 1983]-[Balaban and Tomescu 1989] involved problems associated with polycyclic benzenoids, in particular the definition of isoarithmic cata-condensed benzenoids [Balaban and Tomescu 1983]: they are not only isokekulan (same number K of resonance structures) but, because their 3-digit codes (see further) differ only in the permutation of digits 1 and 2, they have exactly the same electronic properties, in particular there is a one-to-one correspondence between each of their rings.

2 Hidden treasures in Kekulé structures

There is something in common between the Kekulé valence structures and the molecular graphs. At first sight both appear simple and straightforward, if not simplistic, representations of molecules, but in fact both have hidden subtitles that unsuspected onlookers remain mostly unaware of, despite repeated warning to the contrary. About 30 years ago Prelog has written the following mostly overlooked message, just a few months before getting 1975 Nobel Prize in Chemistry, in the Foreword to the book on applications of graph theory to chemistry (edited by one of the present authors), [Balaban 1976]: *Pictorial representations of graphs are so easily intelligible that chemists are often satisfied with inspecting and discussing them without paying too much attention to their algebraic aspects, but it is evident that some familiarity with the theory of graphs is necessary for deeper understanding of their properties.* More recently the other author of this article has written a sizable review on aromaticity in polycyclic conjugated hydrocarbons [Sylvester 1878] which summarizes the fruits of exploring the combinatorial and the topological properties of the Kekulé valence structures, thus emphasizing the point of view of the Discrete Mathematics towards Chemistry, which relates more closely to the valence bond (VB) approach of Quantum Chemistry, rather than to the customary molecular orbital (MO) Quantum Chemistry. The main message of that review was that Kekulé valence structures deserve, even today, much more attention that most chemists have been granting them in the past.

Over 100 years ago, James Joseph Sylvester [Sylvester 1878] the first professor of Mathematics at the Johns Hopkins University and the founder of the *American Journal of Mathematics*, was fascinated by combinatorial and topological properties of Kekulé valence structures, [Kekulé 1865],[Kekulé 1866], which according to him thus opened a novel area of applied mathematics, known as

Graph Theory, [Harary 1969]-[Honsberger 1979]. In fact the term *graph,* for the particular mathematical objects that today form the Graph Theory, has been proposed by Sylvester, and it follows from his interest in Kekuléan diagrams, which represented a chemical graphical notation, from which term *graph* was adopted. Chemists had immediately recognized the merits of Kekulé s structural formula for benzene (extended by Erlenmeyer [Erlenmeyer and Liebigs 1866] to systems of fused benzene rings, and by Bamberger in [Bamberger 1758] and [Bamberger 1893] to aromatic heterocycles) and had acknowledged their appreciation of the significance of this accomplishment by inaugurating its celebration on the occasion of the 25th anniversary of Kekulés paper on the structure of benzene – an event that is not often seen in science, see [Kekulé'25-Conference] and [Borman 1993].

Kekulé structures have played a dominant role in theoretical organic chemistry for over a century and the formed the basis of the early quantum chemical calculations on benzenoid hydrocarbons, initiated by Pauling and Wheland in particular, [Pauling 1939]-[Pauling and Wheland 1933]. The Pauling bond orders [Pauling et al. 1935],[Sedlar et al. 2006] (simply constructed as the ratio between the count for any CC bond – how many times it appears as C=C in the set of K Kekulé valence structures for a benzenoid hydrocarbon – and K) illustrate one of the hidden treasures of Kekulé valence structures. However, despite the considerable attention that Kekulé valence structures received over this long history, few people suspected that there may be additional treasures hidden in Kekulé valence structures that had to be yet discovered. And indeed, it took well over 100 years for new additional interesting and intriguing properties of Kekulé valence structures to surface, [Balaban 1980]-[Klein and Randić 1987] We have summarized in Table 1 several of these relatively recent (in view of the long history of Kekulé valence structures) hidden treasures of Kekulé valence structures. One of the latest of these is the π-electron ring partitions – quantities that bear some conceptual similarity to the celebrated Pauling bond orders, [Randić 2004a],[Randić 2004b].

3 The π-electron ring partition for rings of benzenoids

The π-electron ring partition assigns to each ring of benzenoid hydrocarbons a portion of all π-electrons of the molecule, such that when the total π-content of all rings is counted, one obtains the number N of the π-electrons of the system. Each C=C bond carries two π-electrons which are assigned to a ring if this C=C bond is not shared with adjacent rings, otherwise it contributes a single π-electron to the ring. For each ring, contributions arising from all individual Kekulé valence structures (resonance structures) are added and the total is divided by the number K of Kekulé valence structures in order to obtain

No.	**Treasure**	**Relates to**	**Reference**
1	Pauling bond orders	Bond order-Bond length relationship	Pauling [Pauling 1939]
2	Clar valence structure	Aromatic π-sextet; $6n$ π-electrons rule	Clar [Clar 1972]
3	Conjugated circuits	$4n+2$ and $2n$ rules for aromaticity;Resonance energy expressions	Randić [Randić 1976] -[Randić 2004b]
4	Innate degree of freedom	For solving the inverse Clar structures problem	Randić, Klein [Randić and Klein 1985], [Klein and Randić 1987]
5	The count of all conjugated circuits	Single Kekulé structure has information on all Kekulé structures	Gutman, Randić [Gutman and Randić 1979], cite42
6	Numerical Kekulé valence structures	π-Electron ring partition	Randić, Balaban [Randić and Balaban 2004a] -[Gutman et al. 2005]
7	Numerical benzenoid formula, ring signature	Partitioning of the π-electron ring	Randić, Balaban [Randić and Balaban a], [Randić and Balaban b]

The hidden “treasures” of Kekulé valence structures of conjugated systems

Table 1: The *treasures* of Kekulé valence structures

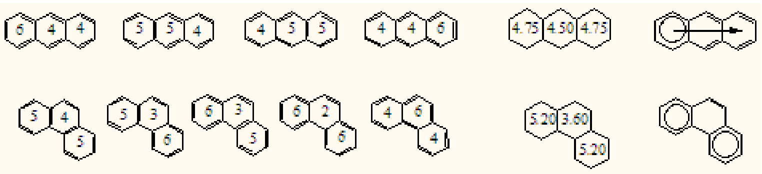
the π-electron ring π-electron partition for this ring. Thus one can associate with each polycyclic conjugated hydrocarbon *a single numerical* Kekulé valence structure, which may replace *the set of K geometrical* Kekulé valence structures.

In a series of papers, [Randić and Balaban 2004a]-[Gutman et al. 2005], the present authors and collaborators have examined many benzenoid and non-benzenoid conjugated hydrocarbons and reported on a number of regularities for the π-electron ring contents. For example, the rings associated with Clars aromatic π-electron sextets show larger π-ring partitions, the rings involving migrating sextets have intermediate π-ring partitions, and the so-called empty rings of Clar have the smallest values of the π-ring content. In passing, one should mention that Gutman showed how in some benzenoids from the perylene family, the empty rings have a substantial π-electron contribution, [Gutman et al. 2004a]. Similarly, the terminal rings in cata-condensed benzenoids have larger π-electron ring partitions.

In this article we look into structural explanations for these earlier observed regularities. Our tool for exploring the structural origin of π-ring partitions is to count the *distribution* of the ring partitions themselves! Specifically, we count how many of the seven possible *types* of benzene rings contribute to each particular ring partition. As different benzenoid ring types we consider benzenoid rings contributing with different numbers of π-electrons to the ring, which can vary from six (for terminal rings of cata-condensed benzenoids) to zero (for a central branching ring, such as the central ring of triphenylene, 4). As is not uncommon in theoretical studies, although we set a well defined goal as the object of our explorations, we obtain as a bonus an unexpected result: a unique characterization of a benzenoid molecule as a whole solely based on partitioning of π-electrons to its rings. This is an interesting result which deserves attention and which by its elegance (or beauty) may qualify to be added as entry 7 to Table 1 as an additional and the latest treasure hidden in Kekulé valence structures for so many years.

4 Partitions of π-electrons in benzenoids

Whereas all cata-condensed benzenoids (catafusenes) with the same number h of hexagonal rings are isomeric, this is not the case for perifusenes, whose molecular formulas depend also on the number a of internal carbon atoms. Catafusenes have $a = 0$. Their notation 3-digit notation consists in 0 (for linear condensation as in 1) and 1 or 2 or kinked condensation (as in 2), provided that the resulting number from sequential listing of these digits is the smallest possible, [Balaban and Harary 1968]-[Balaban et al. 1986]. A non-branched catafusene whose notation has no zero is a fibonacene, [Balaban 1989]. For benzenoids that are stable molecules, a must be an even number, otherwise there can be no Kekuléan resonance structure, and the corresponding benzenoid is an unstable free radical. A benzenoid with h hexagonal rings has molecular formula $C4_{h+2-a}H_{2h+4-a}$. Since each carbon atom contributes with one non-hybridized π-electron to the total number of delocalized electrons of the benzenoid, we denote this number by P. With the above convention for the partition of electrons among benzenoid rings, it is easy to convert geometrical structures of benzenoid rings (individual resonance formulas or Kekulé valence structures) into numerical ones. For the two catafusenes 2 and 3, both of which have 14 π-electrons, the result is presented in Fig. 1. One can see that in both cases the marginal rings are ricer in π-electrons than the middle ring, but for phenanthrene this unequal distribution is more pronounced than in anthracene. Eric Clar proposed a theory illustrating with sextet of π-electron circles an uneven π-electron distribution, and the corresponding Clar structures are presented as the right-most formulas of Fig. 3. The arrow illustrates Clars migrating π-electron sextet. The unique double bond of phenanthrene in the Clar formula is indeed shorter than all other bonds, which is also in agreement with the Pauling bond order.



The π-electron partition between rings resulting from the four resonance structures of anthracene (upper row) and the five resonance structures of phenanthrene (lower row).

Figure 3: The π-electron partition between rings

No.	h	K	Ring	Partition	R_6	R_5	R_4	R_3	R_2	R_1	R_0
2	3	4	AA	4.75	1	1	2	0	0	0	0
		4	B	4.50	0	2	2	0	0	0	0
				12	**2**	**4**	**6**	**0**	**0**	**0**	**0**
3	3	5	AA	5.20	2	2	1	0	0	0	0
		5	B	3.60	1	0	1	2	1	0	0
				15	**5**	**4**	**3**	**2**	**1**	**0**	**0**

For anthracene (2) and phenanthrene (3), the first two lines contain p_{ij} values, and the third line (boldface) provides h, K and R_i values.

Table 2: p_{ij}, h, K, R_i values for anthracene and phenanthrene

In Table 2 we present in a different form the information conveyed by Fig. 3. The number of Kekulé structures is denoted by K, and the rings are designed by capital letters starting with A for the marginal rings. Entries p_{ij} in columns 6 through 12 (where j corresponds to the row number for each type of ring) indicate for each ring how many times this ring is assigned 6 through 0 π-electrons in all K resonance structures. Then relationships (1) – (4) hold for partitions P_j and other numbers from Table 2.

$$P_j = \sum_i i p_{ij}/K \tag{1}$$
$$\sum_j P_j = P = 4h + 2 - a \tag{2}$$
$$\sum_j p_{ij} = R_i \tag{3}$$
$$\sum_i R_i = hK \tag{4}$$

The sequence of Ri numbers, which are indicated in boldface characters on the last row for each benzenoid, can be converted into another sequence that we call the ri sequence, by division with the K value. Then the ri sequence serves for obtaining finally the si sequence or the signature of the benzenoid, according

No.	h	K	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	s_6	s_5	s_4	s_3	s_2	s_1
2	3	4	2	4	6	0	0	0	0	0.5	1.0	1.5	0.0	0.0	0.0	0.0	3.0	5.0	6.0	0.0	0.0	0.0
3	3	5	5	4	3	2	1	0	0	1.0	0.8	0.6	0.4	0.2	0.0	0.0	6.0	4.0	2.4	1.2	0.4	0.0

The R_i, r_i, and s_i sequences for anthracene (2) and phenanthrene (3).

Table 3: R_i, r_i, s_i sequences for anthracene and phenanthrene

to relationships (5) – (8).

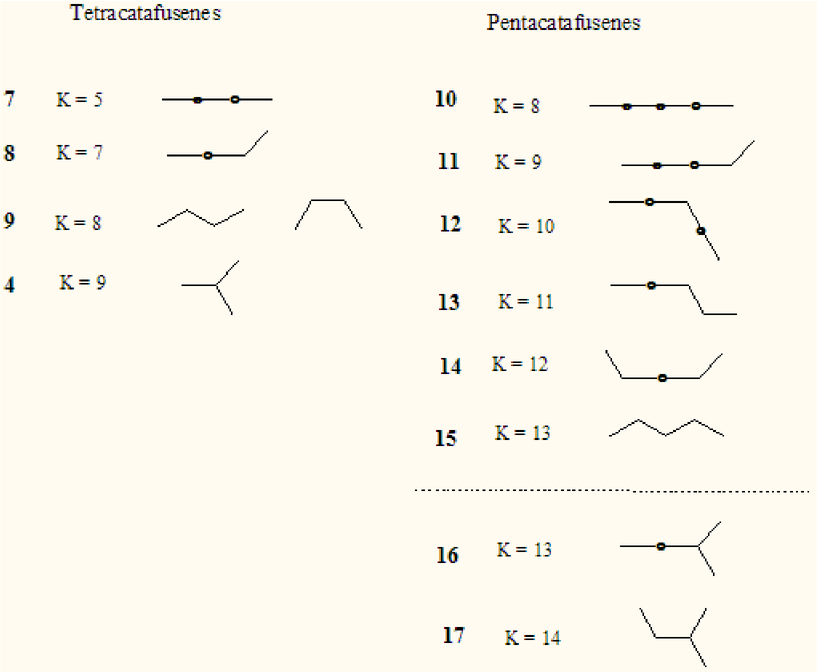
$$r_i = R_i/K \tag{5}$$
$$\textstyle\sum_i r_i = h \tag{6}$$
$$s_i = ir_i \tag{7}$$
$$\textstyle\sum_i s_i = P \tag{8}$$

Thus, we obtain the total number P of π-electrons from entries p_{ij} of Table 2 in two different ways: from the row sums providing the partition, and from the column sums providing the signature. Table 3 summarizes for 2 and 3 the above relationships.

For exemplifying better the partitions of π-electrons we shall use catafusenes and perifusenes with four to six benzenoid rings, and when several isoarithmic systems exist, we shall discuss only one of them. In the following section, after the model of anthracene and phenanthrene, the structures of catafusenes will be described by means of their dualists, whereas perifusenes will be shown with their rings.

In Fig. 4 one can see on the left-hand side the dualists of all five possible tetracatafusenes. There are two isoarithmic tetracatafusenes with $K = 8$ resonance structures, having notation [12] and [11], respectively; from them, only one denoted as 9, will be included in the following discussion because their electronic properties are identical (no other isoarithmic benzenoids will be shown henceforth). On the right-hand side are presented dualists of pentacatafusenes, with rings denoted by capital letters starting from one endpoint (vertex with degree 1); non-branched catafusenes 10 – 15 are on top and two branched catafusenes (16, 17) follow. Fig. 5 contains on the left-hand side non-branched hexacatafusenes and branched isomers on the right-hand side. The R_i sequences for all catafusenes and their partitions are presented in Table 4. The ordering of benzenoids follows increasing K values, and in Tables 4 and 5 the notation with boldface numbers is not always in agreement with this ordering because we separate in figures and tables the branched from the non-branched catafusenes, and perifusenes with two internal vertices from those with four internal vertices.

Structures of perifusenes with $h = 5$ and 6 benzenoid rings are shown in Fig. 6. Table 5 contains partitions Pi and Ri sequences for non-isoarithmic perifusenes

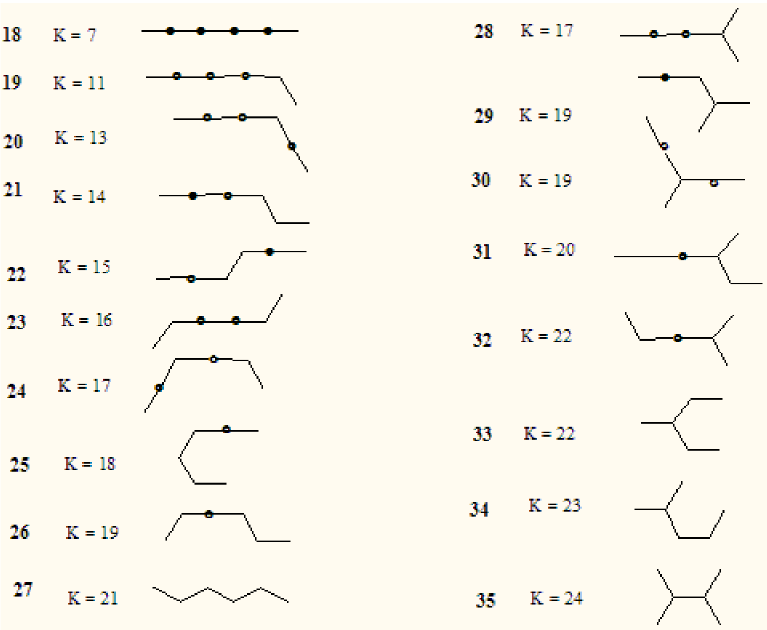


Dualists of tetracatafusenes (left-hand part) and pentacatafusenes (right-hand part, with non-branched systems above the dotted line and branched isomers below it).

Figure 4: Dualists of tetracatafusenes and pentacatafusenes

with $h = 4$, 5, and 6 benzenoid rings.

For catafusenes with 4, 5, and 6 benzenoid rings, in Table 6 we repeat in columns 4 – 10 the R_i sequence (its row sum is hK), then the r_i sequence (its row sum is h), and in columns 18 – 23 the si sequence (its row sum is P, the number of π-electrons and carbon atoms). The next column labeled $z + 1$ indicates one plus the number of zeros in the 3-digit notation (it was found that this is a simple parameter correlating with many properties of catafusenes). The last three columns indicate pairwise sums among terms in the si sequence, whose importance will be discussed in the next section. A similar presentation follows in Table 7 for perifusenes with 4, 5, and 6 benzenoid rings, with the difference that instead of the column with $z+1$ values one has a column with the number P of π-electrons (kekuléan tetraperifusenes and pentaperifusenes can have only two internal vertices, but hexaperifusenes can have either 2 or 4 internal vertices).

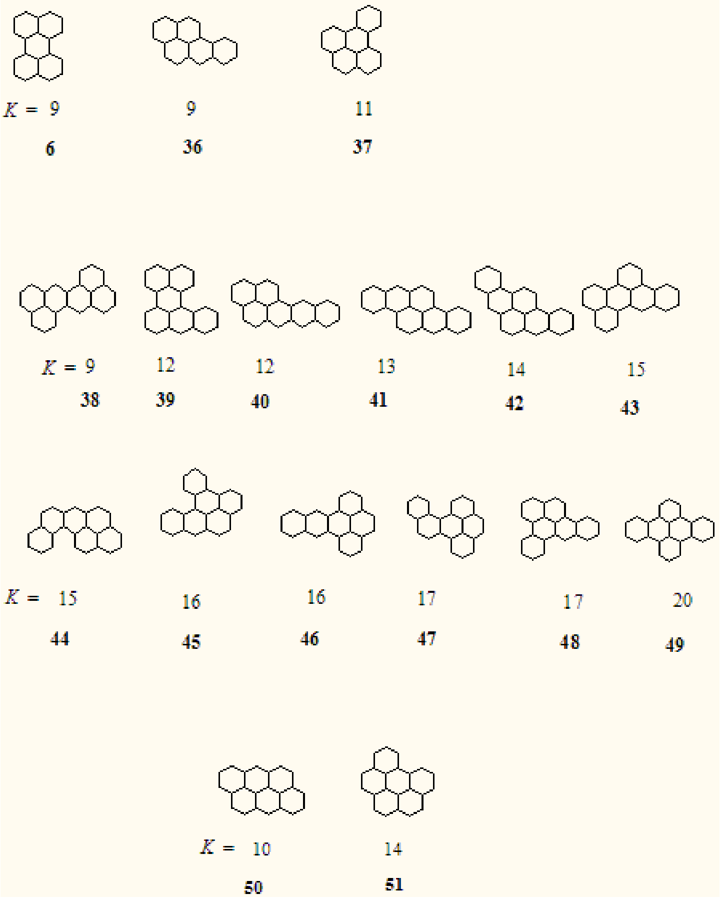


Dualists of non-branched (left-hand part) and branched (right-hand part) of hexacatafusenes.

Figure 5: Dualists of non-branched and branched hexacatafusenes

5 A new metric for benzenoids based on sums from their signature

An interesting observation is that for isomeric haxacatafusenes or hexaperifusenes there is a good correlation between the sums $s_6 + s_5$ and $s_4 + s_3$ as seen in Figures 7 and 8. The non-branched catafusenes are grouped at the top left half of the straight line, while the branched isomers are on the lower right of that line. A perfectly linear correlation with slope –1 exists between the sums $S_1 = s_6 + s_5 + s_2 + s_1$ and $S_2 = s_4 + s_3$, based on their si sequence. Among other possible divisions of P into two unequal parts, this seems to be the best one. This means that the $P(= S1 + S2)$ π-electrons are divided between these two sums, with the $S1$-rich and $S2$-poor benzenoids having many Clar sextets, whereas systems with few Clar sextets have low $S1$ values and high $S2$ values. Systems with many Clar sextets have a high branching degree (which increases the numbers composing $S1$ and decreases the numbers composing $S2$). Systems with few Clar sextets (such as acenes or perifusenes with long acenic tails arranged in just a few horizontal layers of rings) have high $S2$ values and low $S1$ values.



Structures of non-isoarithmic pentaperifusenes (top row) and hexaperifusenes with two internal vertices (2nd and 3rd rows) or four internal carbon atoms (bottom row).

Figure 6: Structures of non-isoarithmic pentaperifusenes and hexaperifusenes

There is a very approximate linear correlation between $S1$ and the number K of Kekulé structures. Whereas K values have a fairly high degeneracy, the sums $S1$ and $S2$ have a very low degeneracy. Ordering of benzenoids by K values is imprecise, but now we have a new metric involving a much better sorting criterion based on these sums. Of course, there is no disagreement between sorting by $S1$ and $S2$. This ordering provides a reliable classification of isomeric benzenoids, with very low degeneracy, allowing a closer insight into their complexity.

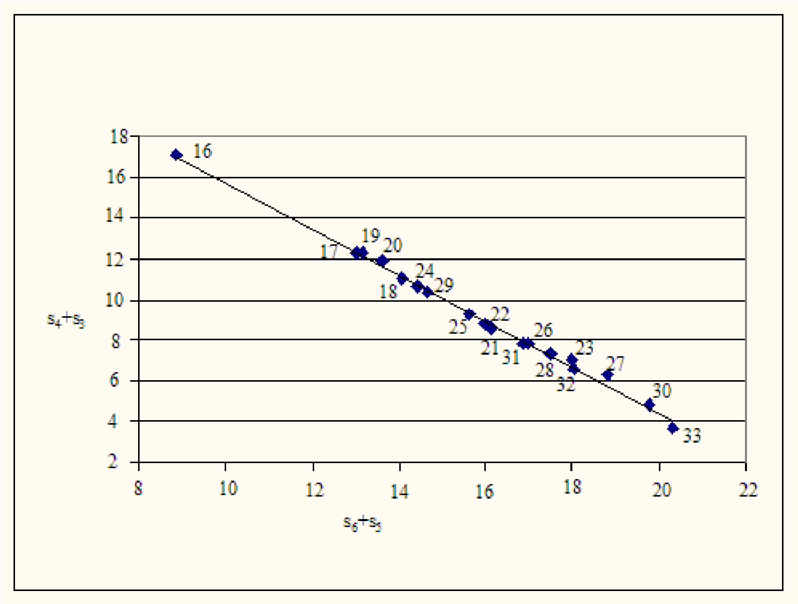


Figure 7: Plot of s4+s3 versus s6+s5 for hexacatafusenes

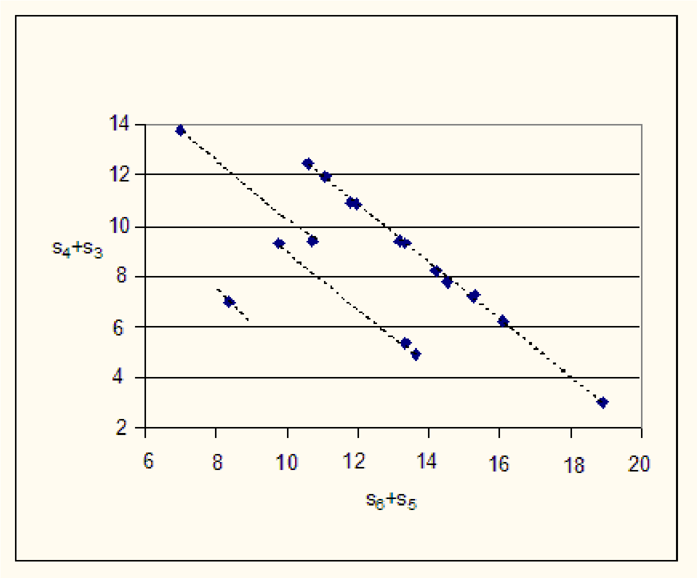


Figure 8: Plot of perifusenes with 4 rings (unique point), 5 rings (three points), 6 rings with four internal carbons (two points) and 6 rings with two internal carbons (right-most line)

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Appendix: Tables

No.	h	K	Ring	Partition	R_6	R_5	R_4	R_3	R_2	R_1	R_0
7	4	5	AA	4.600	1	1	3	0	0	0	0
			BB	4.400	0	2	3	0	0	0	0
				20	2	6	12	0	0	0	0
8	4	7	AA	4.857	2	2	3	0	0	0	0
			B	4.571	0	4	3	0	0	0	0
			C	3.286	1	0	1	3	2	0	0
			D	5.286	3	3	1	0	0	0	0
				28	6	9	8	3	2	0	0
9	4	8	AA	5.125	3	3	2	0	0	0	0
			BB	3.875	2	0	2	3	1	0	0
				32	10	6	8	6	2	0	0
4	4	9	AAA	5.333	4	4	1	0	0	0	0
			B	2.000	1	0	0	1	3	3	1
				36	13	12	3	1	3	3	1
10	5	6	AA	4.500	1	1	4	0	0	0	0
			BB	4.333	0	2	4	0	0	0	0
			C	5.167	0	3	4	0	0	0	0
				30	2	8	20	0	0	0	0
11	5	9	A	4.667	2	2	5	0	0	0	0
			B	4.444	0	4	5	0	0	0	0
			C	4.444	0	4	5	0	0	0	0
			D	3.111	1	0	1	4	3	0	0
			E	5.333	4	4	1	0	0	0	0
				45	7	14	17	4	3	0	0
12	5	10	AA	4.000	3	3	4	0	0	0	0
			BB	4.600	0	6	4	0	0	0	0
			C	3.000	1	0	1	4	4	0	0
				50	7	18	17	4	4	0	0
13	5	11	A	4.818	3	3	5	0	0	0	0
			B	12.500	0	6	5	0	0	0	0
			C	3.545	2	0	2	5	2	0	0
			D	4.000	3	0	3	4	1	0	0
			E	5.091	4	4	3	0	0	0	0
				55	12	13	18	9	3	0	0
14	5	12	AA	5.250	5	5	2	0	0	0	0
			BB	3.417	2	0	2	5	3	0	0
			C	4.667	0	8	4	0	0	0	0
				60	14	18	12	10	6	0	0
15	5	13	AA	5.154	5	5	3	0	0	0	0
			BB	3.769	3	0	3	5	2	0	0
			C	4.154	4	0	4	4	1	0	0
				65	20	10	16	14	5	0	0

Table 4: Partitions and Ri sequences for catafusenes with h = 4,5,6 rings

No.	h	K	Ring	Partition	R_6	R_5	R_4	R_3	R_2	R_1	R_0
16	5	13	A	4.923	4	4	5	0	0	0	0
			B	4.615	0	8	5	0	0	0	0
			C	1.692	1	0	0	1	4	5	2
			DD	5.385	6	6	1	0	0	0	0
				65	17	24	12	1	4	5	2
17	5	14	A	5.071	5	5	4	0	0	0	0
			B	4.071	4	0	4	5	1	0	0
			C	2.286	2	0	0	2	5	4	1
			D	5.286	6	6	2	0	0	0	0
			E	5.286	6	6	2	0	0	0	0
				70	23	17	12	7	6	4	1
18	6	7	AA	4.429	1	1	5	0	0	0	0
			BB	4.286	0	2	5	0	0	0	0
			CC	4.286	0	2	5	0	0	0	0
				42	2	10	30	0	0	0	0
19	6	11	A	4.545	2	2	7	0	0	0	0
			B	4.364	0	4	7	0	0	0	0
			C	4.364	0	4	7	0	0	0	0
			D	4.364	0	4	7	0	0	0	0
			E	3.000	1	0	1	5	4	0	0
			F	5.364	5	5	1	0	0	0	0
				66	8	19	30	5	4	0	0
20	6	13	A	4.692	3	3	7	0	0	0	0
			B	4.462	0	6	7	0	0	0	0
			C	4.462	0	6	7	0	0	0	0
			D	2.846	1	0	1	5	6	0	0
			E	4.615	0	8	5	0	0	0	0
			F	4.923	4	4	5	0	0	0	0
				78	8	27	32	5	6	0	0
21	6	14	A	4.643	3	3	8	0	0	0	0
			B	4.429	0	6	8	0	0	0	0
			C	4.429	0	6	8	0	0	0	0
			D	3.357	2	0	2	7	3	0	0
			E	4.071	4	0	4	5	1	0	0
			F	5.071	5	5	4	0	0	0	0
				84	14	20	34	12	4	0	0
22	6	15	AA	4.800	4	4	7	0	0	0	0
			BB	4.533	0	8	7	0	0	0	0
			CC	3.667	3	0	3	7	2	0	0
				90	14	24	34	14	4	0	0
23	6	16	AA	5.313	7	7	2	0	0	0	0
			BB	3.188	2	0	2	7	5	0	0
			CC	4.500	0	8	8	0	0	0	0
				96	18	30	24	14	10	0	0

Table 4: Partitions and Ri ... (cont.)

No.	h	K	Ring	Partition	R_6	R_5	R_4	R_3	R_2	R_1	R_0
24	6	17	A	4.882	5	5	7	0	0	0	0
			B	4.588	0	10	7	0	0	0	0
			C	3.118	2	0	2	7	6	0	0
			D	4.706	0	12	5	0	0	0	0
			E	3.471	3	0	3	7	4	0	0
			F	5.235	7	7	3	0	0	0	0
				102	17	34	27	14	10	0	0
28	6	17	A	4.706	4	4	9	0	0	0	0
			B	4.471	0	8	9	0	0	0	0
			C	4.471	0	8	9	0	0	0	0
			D	1.529	1	0	0	1	5	7	3
			E	5.412	8	8	1	0	0	0	0
			F	5.412	8	8	1	0	0	0	0
				102	21	36	29	1	5	7	3
25	6	18	A	4.833	5	5	8	0	0	0	0
			B	4.556	0	10	8	0	0	0	0
			C	3.444	3	0	3	8	4	0	0
			D	4.278	6	0	6	5	1	0	0
			E	3.722	4	0	4	7	3	0	0
			F	5.167	7	7	4	0	0	0	0
				108	25	22	33	20	8	0	0
26	6	19	A	5.105	7	7	5	0	0	0	0
			B	3.947	5	0	5	7	2	0	0
			C	3.684	4	0	4	8	3	0	0
			D	4.632	0	12	7	0	0	0	0
			E	3.368	3	0	3	8	5	0	0
			F	5.263	8	8	3	0	0	0	0
				114	27	27	27	23	10	0	0
29	6	19	A	4.789	5	5	9	0	0	0	0
			B	4.526	0	10	9	0	0	0	0
			C	3.737	4	0	4	9	2	0	0
			D	2.421	3	0	0	3	7	5	1
			E	5.263	8	8	3	0	0	0	0
			F	5.263	8	8	3	0	0	0	0
				114	28	31	28	12	9	5	1
30	6	19	AA	4.947	6	6	7	0	0	0	0
			BB	4.632	0	12	7	0	0	0	0
			C	1.421	1	0	0	1	5	8	4
			D	5.421	9	9	1	0	0	0	0
				114	22	45	29	1	5	8	4
31	6	20	A	4.900	6	6	8	0	0	0	0
			B	4.600	0	12	8	0	0	0	0
			C	1.900	2	0	0	2	7	6	3
			D	5.350	9	9	2	0	0	0	0
			E	4.150	6	0	6	7	1	0	0
			F	5.050	7	7	6	0	0	0	0
				120	30	34	30	9	8	6	3

Table 4: Partitions and Ri ... (cont.)

No.	h	K	Ring	Partition	R_6	R_5	R_4	R_3	R_2	R_1	R_0
27	6	21	AA	5.143	8	8	5	0	0	0	0
			BB	3.810	5	0	5	8	3	0	0
			CC	4.048	6	0	6	7	2	0	0
				126	38	16	32	30	10	0	0
32	6	22	A	5.227	9	9	4	0	0	0	0
			B	3.500	4	0	4	9	5	0	0
			C	4.727	0	16	6	0	0	0	0
			D	1.818	2	0	0	2	7	8	3
			E	5.364	10	10	2	0	0	0	0
			F	5.364	10	10	2	0	0	0	0
				132	35	45	18	11	12	8	3
33	6	22	AA	5.091	8	8	6	0	0	0	0
			BB	4.000	6	0	6	8	2	0	0
			C	2.591	4	0	0	4	8	5	1
			D	5.227	9	9	4	0	0	0	0
				132	41	25	28	20	12	5	1
34	6	23	A	5.714	9	9	5	0	0	0	0
			B	3.696	5	0	5	9	4	0	0
			C	4.348	8	0	8	6	1	0	0
			D	2.174	3	0	0	3	8	7	2
			E	5.304	10	10	3	0	0	0	0
			F	5.304	10	10	3	0	0	0	0
				138	45	29	24	18	13	7	2
35	6	24	$AAAA$	5.250	10	10	4	0	0	0	0
			BB	2.500	4	0	0	4	9	6	1
				144	48	40	16	8	18	12	2

Table 4: Partitions and Ri ... (cont.)

h	No.	K	$ring$	$P_i; K_h$	R_6	R_5	R_4	R_3	R_2	R_1	R_0
4	5	6	$A(2)$	4.667	0	4	2	0	0	0	0
			$B(2)$	3.333	0	1	1	3	1	0	0
				24	0	10	6	6	2	0	0
5	6	9	$A(4)$	4.667	0	6	3	0	0	0	0
			B	1.333	0	0	0	0	4	4	1
				45	0	24	12	0	4	4	1
5	36	9	A	5.000	3	3	3	0	0	0	0
			B	3.667	0	2	3	3	1	0	0
			C	3.11	0	1	1	5	2	0	0
			D	4.667	0	6	3	0	0	0	0
			E	3.56	0	2	2	4	1	0	0
				45	3	14	12	12	4	0	0
5	37	11	A	5.36	5	5	1	0	0	0	0
			B	1.82	0	1	0	1	4	4	1
			$C(2)$	4.73	0	8	3	0	0	0	0
			D	3.36	0	2	2	5	2	0	0
				55	5	24	9	6	6	4	1
6	38	9	$A(2)$	2.667	0	6	3	0	0	0	0
			$B(2)$	4.667	0	6	3	0	0	0	0
			$C(2)$	4.667	0	0	0	6	3	0	0
				54	0	24	12	12	6	0	0
6	39	10	$A(2)$	4.600	0	6	4	0	0	0	0
			$B(2)$	3.300	0	0	4	5	1	0	0
			$C(2)$	3.100	0	1	1	6	2	0	0
				60	0	14	18	22	6	0	0
6	40	12	A	4.750	3	3	6	0	0	0	0
			B	4.000	0	3	6	3	0	0	0
			C	4.500	0	6	6	0	0	0	0
			D	1.42	0	0	0	0	6	5	1
			E	4.667	0	8	4	0	0	0	0
			F	4.667	0	8	4	0	0	0	0
				72	3	28	26	3	6	5	1
6	41	12	A	4.750	3	3	6	0	0	0	0
			B	4.500	0	6	6	0	0	0	0
			C	3.42	0	2	3	5	2	0	0
			D	3.000	0	1	1	7	3	0	0
			E	4.667	0	8	4	0	0	0	0
			F	3.667	0	3	3	5	1	0	0
				72	3	23	23	17	6	0	0
6	42	13	$A(2)$	4.923	4	4	5	0	0	0	0
			$B(2)$	3.769	0	3	5	4	1	0	0
			$C(2)$	3.307	0	2	2	7	2	0	0
				78	8	18	24	22	6	0	0
6	43	14	$A(2)$	5.071	5	5	4	0	0	0	0
			$B(2)$	3.571	0	3	4	5	2	0	0
			C	2.929	0	1	1	8	4	0	0
			D	3.786	0	4	4	5	1	0	0
				84	10	21	21	23	9	0	0

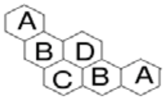

Table 5: Structures, partitions P_i, entries p_{ij}, and R_i sequences of perifusenes with h = 4, 5, and 6

h	No.	K	$ring$	$P_i; K_h$	R_6	R_5	R_4	R_3	R_2	R_1	R_0
6	44	14	$A(2)$	4.714	0	10	4	0	0	0	0
			$B(2)$	3.500	0	3	3	6	2	0	0
			C	3.857	0	4	5	4	1	0	0
			D	1.714	0	0	1	1	6	5	1
				84	0	30	20	17	11	5	1
6	45	15	A	5.200	6	6	5	0	0	0	0
			B	3.400	0	3	3	6	3	0	0
			C	4.800	0	12	3	0	0	0	0
			D	1.264	0	0	0	0	6	7	2
			E	4.678	0	10	5	0	0	0	0
			F	4.678	0	10	5	0	0	0	0
				90	6	41	19	6	9	7	2
6	46	15	A	5.200	6	6	3	0	0	0	0
			B	3.600	3	0	3	6	3	0	0
			C	3.867	0	4	6	4	1	0	0
			D	3.200	0	2	2	8	3	0	0
			E	3.467	0	3	3	7	2	0	0
			F	4.667	0	10	5	0	0	0	0
				90	9	25	22	25	9	0	0
6	47	16	A	4.938	5	5	6	0	0	0	0
			B	3.813	0	4	6	5	1	0	0
			C	3.125	0	2	2	8	4	0	0
			D	4.750	0	12	4	0	0	0	0
			E	2.063	0	2	0	2	6	5	1
			F	5.313	7	7	2	0	0	0	0
				96	12	32	20	15	11	5	1
6	48	16	A	4.938	5	5	6	0	0	0	0
			B	4.625	0	10	6	0	0	0	0
			C	1.563	0	1	0	1	5	7	2
			D	3.375	0	3	3	7	3	0	0
			$E(2)$	4.750	0	12	4	0	0	0	0
				96	5	43	23	8	8	7	2
6	49	17	A	5.059	6	6	5	0	0	0	0
			B	4.118	5	0	5	6	1	0	0
			C	2.059	0	2	0	2	7	5	1
			$D(2)$	4.706	0	12	5	0	0	0	0
			E	3.353	0	3	3	8	3	0	0
				102	11	35	23	16	11	5	1
6	50	17	A	5.059	6	6	5	0	0	0	0
			B	3.647	0	4	5	6	2	0	0
			C	3.588	0	4	4	7	2	0	0
			D	4.706	0	12	5	0	0	0	0
			E	1.706	0	1	0	1	6	7	2
			F	5.412	8	8	1	0	0	0	0
				102	14	35	20	14	10	7	2
6	51	20	$A(2)$	5.350	9	9	2	0	0	0	0
			$B(2)$	1.850	0	2	0	2	7	7	2
			$C(2)$	4.800	0	16	4	0	0	0	0
				120	18	54	12	4	14	14	4

Table 5: Structures, partitions P_i ... (cont.)

$No.$	h	K	$R6$	$R5$	$R4$	$R3$	$R2$	$R1$	$R0$	$r6$	$r5$	$r4$	$r3$	$r2$	$r1$	$r0$	...
4	4	5	2	6	12	0	0	0	0	0.400	1.200	2.400	0.000	0.000	0.000	0.000	...
5	4	7	6	9	8	3	2	0	0	0.857	1.286	1.143	0.429	0.286	0.000	0.000	...
6	4	8	10	6	8	6	2	0	0	1.250	0.750	1.000	0.750	0.250	0.000	0.000	...
7	4	9	13	12	3	1	3	3	1	1.444	1.333	0.333	0.111	0.333	0.333	0.111	...
8	5	6	2	8	20	0	0	0	0	0.333	1.333	3.333	0.000	0.000	0.000	0.000	...
9	5	9	7	14	17	4	3	0	0	0.778	1.556	1.889	0.444	0.333	0.000	0.000	...
10	5	10	7	18	17	4	4	0	0	0.700	1.800	1.700	0.400	0.400	0.000	0.000	...
11	5	11	12	13	18	9	3	0	0	1.091	1.182	1.636	0.818	0.273	0.000	0.000	...
12	5	12	14	18	12	10	6	0	0	1.167	1.500	1.000	0.833	0.500	0.000	0.000	...
13	5	13	20	10	16	14	5	0	0	1.538	0.769	1.231	1.077	0.385	0.000	0.000	...
14	5	13	17	24	12	1	4	5	2	1.308	1.846	0.923	0.077	0.308	0.385	0.154	...
15	5	14	23	17	12	7	6	4	1	1.643	1.214	0.857	0.500	0.429	0.286	0.071	...
16	6	7	2	10	30	0	0	0	0	0.286	1.429	4.286	0.000	0.000	0.000	0.000	...
17	6	11	8	19	30	5	4	0	0	0.727	1.727	2.727	0.455	0.364	0.000	0.000	...
18	6	13	8	27	32	5	6	0	0	0.615	2.077	2.462	0.385	0.462	0.000	0.000	...
19	6	14	14	20	34	12	4	0	0	1.000	1.429	2.429	0.857	0.286	0.000	0.000	...
20	6	15	14	24	34	14	4	0	0	0.933	1.600	2.267	0.933	0.267	0.000	0.000	...
21	6	16	18	30	24	14	10	0	0	1.125	1.875	1.500	0.875	0.625	0.000	0.000	...
22	6	17	17	34	27	14	10	0	0	1.000	2.000	1.588	0.824	0.588	0.000	0.000	...
23	6	17	21	36	29	1	5	7	3	1.235	2.118	1.706	0.059	0.294	0.412	0.176	...
24	6	18	25	22	33	20	8	0	0	1.389	1.222	1.833	1.111	0.444	0.000	0.000	...
25	6	19	27	27	27	23	10	0	0	1.421	1.421	1.421	1.211	0.526	0.000	0.000	...
26	6	19	28	31	28	12	9	5	1	1.474	1.632	1.474	0.632	0.474	0.263	0.053	...
27	6	19	22	45	29	1	5	8	4	1.158	2.368	1.526	0.053	0.263	0.421	0.211	...
28	6	20	30	34	30	9	8	6	3	1.500	1.700	1.500	0.450	0.400	0.300	0.150	...
29	6	21	38	16	32	30	10	0	0	1.810	0.762	1.524	1.429	0.476	0.000	0.000	...
30	6	22	35	45	18	11	12	8	3	1.591	2.045	0.818	0.500	0.545	0.364	0.136	...
31	6	22	41	25	28	20	12	5	1	1.864	1.136	1.273	0.909	0.545	0.227	0.045	...
32	6	23	45	29	24	18	13	7	2	1.957	1.261	1.043	0.783	0.565	0.304	0.087	...
33	6	24	48	40	16	8	18	12	2	2.000	1.667	0.667	0.333	0.750	0.500	0.083	...

Table 6: Sequences for catafusenes with h = 4,5,6 rings.

...	$s6$	$s5$	$s4$	$s3$	$s2$	$s1$	$z+1$	$s6+s5$	$s4+s3$	$s6521$	$No.$
...	2.400	6.000	9.600	0.000	0.000	0.000	3	8.400	9.600	8.400	4
...	5.143	6.429	4.571	1.286	0.571	0.000	2	11.572	5.857	12.143	5
...	7.500	3.750	4.000	2.250	0.500	0.000	1	11.250	6.250	11.750	6
...	8.667	6.667	1.333	0.333	0.667	0.333	1	15.334	1.666	16.334	7
...	2.000	6.667	13.333	0.000	0.000	0.000	4	8.667	13.333	8.667	8
...	4.667	7.778	7.556	1.333	0.667	0.000	3	12.445	8.889	13.112	9
...	4.200	9.000	6.800	1.200	0.800	0.000	3	13.200	8.000	14.000	10
...	6.545	5.909	6.545	2.455	0.545	0.000	2	12.454	9.000	12.999	11
...	7.000	7.500	4.000	2.500	1.000	0.000	2	14.500	6.500	15.500	12
...	9.231	3.846	4.923	3.231	0.769	0.000	1	13.077	8.154	13.846	13
...	7.846	9.231	3.692	0.231	0.615	0.385	2	17.077	3.923	18.077	14
...	9.857	6.071	3.429	1.500	0.857	0.286	1	15.928	4.929	17.071	15
...	1.714	7.143	17.143	0.000	0.000	0.000	5	8.857	17.143	8.857	16
...	4.364	8.636	10.909	1.364	0.727	0.000	4	13.000	12.273	13.727	17
...	3.692	10.385	9.846	1.154	0.923	0.000	4	14.077	11.000	15.000	18
...	6.000	7.143	9.714	2.571	0.571	0.000	3	13.143	12.285	13.714	19
...	5.600	8.000	9.067	2.800	0.533	0.000	3	13.600	11.867	14.133	20
...	6.750	9.375	6.000	2.625	1.250	0.000	3	16.125	8.625	17.375	21
...	6.000	10.000	6.353	2.471	1.176	0.000	3	16.000	8.824	17.176	22
...	7.412	10.588	6.824	0.176	0.588	0.412	3	18.000	7.000	19.000	23
...	8.333	6.111	7.333	3.333	0.889	0.000	2	14.444	10.666	15.333	24
...	8.526	7.105	5.684	3.632	1.053	0.000	2	15.631	9.316	16.684	25
...	8.842	8.158	5.895	1.895	0.947	0.263	2	17.000	7.790	18.210	26
...	6.947	11.842	6.105	0.158	0.526	0.421	3	18.789	6.263	19.736	27
...	9.000	8.500	6.000	1.350	0.800	0.300	2	17.500	7.350	18.600	28
...	10.857	3.810	6.095	4.286	0.952	0.000	1	14.667	10.381	15.619	29
...	9.545	10.227	3.273	1.500	1.091	0.364	2	19.772	4.773	21.227	30
...	11.182	5.682	5.091	2.727	1.091	0.227	1	16.864	7.818	18.182	31
...	11.739	6.304	4.174	2.348	1.130	0.304	1	18.043	6.522	19.477	32
...	12.000	8.333	2.667	1.000	1.500	0.500	1	20.333	3.667	22.333	33

Table 6: Sequences for catafusenes ... (cont).

$No.$	h	K	$R6$	$R5$	$R4$	$R3$	$R2$	$R1$	$R0$	$r6$	$r5$	$r4$	$r3$	$r2$	$r1$	$r0$	$s6$	$s5$	$s4$	$s3$	$s2$	$s1$	P	$s6+s5$	$s4+s3$	$s6521$
1	4	6	0	10	6	6	2	0	0	0.000	1.667	1.000	1.000	0.333	0.000	0.000	0.000	8.333	4.000	3.000	0.667	0.000	16	8.333	7.000	9.000
2	5	9	0	24	12	0	4	4	1	0.000	2.667	1.333	0.000	0.444	0.444	0.111	0.000	13.333	5.333	0.000	0.889	0.444	20	13.333	5.333	14.666
3	5	9	3	14	12	12	4	0	0	0.333	1.556	1.333	1.333	0.444	0.000	0.000	2.000	7.778	5.333	4.000	0.889	0.000	20	9.778	9.333	10.667
4	5	11	5	24	9	6	6	4	1	0.455	2.182	0.818	0.545	0.545	0.364	0.091	2.727	10.909	3.273	1.636	1.091	0.364	20	13.636	4.909	15.091
5	6	9	0	24	12	12	6	0	0	0.000	2.667	1.333	1.333	0.667	0.000	0.000	0.000	13.333	5.333	4.000	1.333	0.000	24	13.333	9.333	14.666
7	6	12	3	28	26	3	6	5	1	0.250	2.333	2.167	0.250	0.500	0.417	0.083	1.500	11.667	8.667	0.750	1.000	0.417	24	13.167	9.417	14.584
8	6	12	3	23	23	17	6	0	0	0.250	1.917	1.917	1.417	0.500	0.000	0.000	1.500	9.583	7.667	4.250	1.000	0.000	24	11.083	11.917	12.083
9	6	13	8	18	24	22	6	0	0	0.615	1.385	1.846	1.692	0.462	0.000	0.000	3.692	6.923	7.385	5.077	0.923	0.000	24	10.615	12.462	11.538
10	6	14	10	21	21	23	9	0	0	0.714	1.500	1.500	1.643	0.643	0.000	0.000	4.286	7.500	6.000	4.929	1.286	0.000	24	11.786	10.929	13.072
12	6	15	6	41	19	6	9	7	2	0.400	2.733	1.267	0.400	0.600	0.467	0.133	2.400	13.667	5.067	1.200	1.200	0.467	24	16.067	6.267	17.734
13	6	15	9	25	22	25	9	0	0	0.600	1.667	1.467	1.667	0.600	0.000	0.000	3.600	8.333	5.867	5.000	1.200	0.000	24	11.933	10.867	13.133
14	6	16	12	32	20	15	11	5	1	0.750	2.000	1.250	0.938	0.688	0.313	0.063	4.500	10.000	5.000	2.813	1.375	0.313	24	14.500	7.813	16.188
15	6	16	5	43	23	8	8	7	2	0.313	2.688	1.438	0.500	0.500	0.438	0.125	1.875	13.438	5.750	1.500	1.000	0.438	24	15.313	7.250	16.751
16	6	17	11	35	23	16	11	5	1	0.647	2.059	1.353	0.941	0.647	0.294	0.059	3.882	10.294	5.412	2.824	1.294	0.294	24	14.176	8.236	15.764
17	6	17	14	35	20	14	10	7	2	0.824	2.059	1.176	0.824	0.588	0.412	0.118	4.941	10.294	4.706	2.471	1.176	0.412	24	15.235	7.177	16.823
18	6	20	18	54	12	4	14	14	4	0.900	2.700	0.600	0.200	0.700	0.700	0.200	5.400	13.500	2.400	0.600	1.400	0.700	24	18.900	3.000	21.000
6	6	10	0	14	18	22	6	0	0	0.000	1.400	1.800	2.200	0.600	0.000	0.000	0.000	7.000	7.200	6.600	1.200	0.000	22	7.000	13.800	8.200
11	6	14	0	30	20	17	11	5	1	0.000	2.143	1.429	1.214	0.786	0.357	0.071	0.000	10.714	5.714	3.643	1.571	0.357	22	10.714	9.357	12.642

Table 7: Sequences for perifusenes with h = 4, 5, and 6 rings.