

RELATIONS BETWEEN THE PERMANENTAL AND CHARACTERISTIC POLYNOMIALS OF FULLERENES AND BENZENOID HYDROCARBONS

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Abstract

In earlier computer-aided studies the permanental polynomials of numerous fullerenes and benzenoid hydrocarbons were determined. Several relations between the coefficients of the permanental and characteristic polynomials were then observed. We now demonstrate the general validity of these empirically discovered regularities and establish a few more.

INTRODUCTION

Graph polynomials were among the most popular objects of research in chemical graph theory (see, for instance, the monographs [1-4]) and continue to be so until the most recent days (see, for instance, chapter 3 of the book [5] and the references cited therein).

No doubt, the most extensively examined such polynomial is the *characteristic polynomial* $\phi(G)$. It is defined as follows.

Let G be a graph on n vertices and A be its $(0, 1)$ -adjacency matrix [1-3]. Hence A is a square matrix of order n . By I is denoted the unit matrix of order n . The characteristic polynomial of the graph G is, by definition,

$$\phi(G) = \phi(G, \lambda) = \det(\lambda I - A) \quad (1)$$

and we will write it in the coefficient form

$$\phi(G, x) = \sum_{k=0}^n a_k \lambda^{n-k}. \quad (2)$$

The importance of the characteristic polynomial lies in the fact that its zeros are just the eigenvalues of the adjacency matrix, hence the graph eigenvalues, which has noteworthy quantum chemical implications (for details see [3, 4]). Special techniques were developed for the calculation of the coefficients a_k of the characteristic polynomial [5], among which the Sachs theorem plays an outstanding role [6, 7]; see below. From Eq. (1) we see that the characteristic polynomial is the determinant of a certain matrix, namely of $(\lambda I - A)$. For quite some time there is a tendency in chemical graph theory to study graph polynomials other than $\phi(G)$. This lead to the natural idea to apply some other algebraic operators to the matrix $(\lambda I - A)$. The best known such operator is the permanent [8].

Thus, in analogy to Eq. (1), one defines the *permanental polynomial* $\pi(G)$ as

$$\pi(G) = \pi(G, \lambda) = \text{per}(\lambda I - A). \quad (3)$$

In what follows, in parallel to Eq. (2), we write the permanental polynomial in the coefficient form

$$\pi(G, \lambda) = \sum_{k=0}^n b_k \lambda^{n-k}. \quad (4)$$

It seems that the permanental polynomial was considered for the first time in the chemical literature in 1981 by Kasum et al. [9]. The study of analogous objects in the mathematical literature started not much earlier [10]. Nevertheless, permanents and permanental polynomials did not attract much attention of chemical graph-theoreticians [11, 12]. This situation has changed somewhat only recently [13-17]. One of the present authors has recently developed a computer-aided method for the calculation of the permanental polynomial of molecular graphs [15] and applied it to a variety of benzenoid hydrocarbons

[15] and fullerenes [16]. These studies revealed the existence of several relations between the coefficients a_k and b_k of the characteristic and permanental polynomials, Eqs. (2) and (4). In this work we provide formal proofs of the general validity of the regularities empirically discovered in [15, 16] and establish a few more.

At this point it is worth noting that both the determinant and the permanent are special cases of so-called immanants [8]. Consequently, in analogy to Eqs. (1) and (3), a whole class of “immanantal polynomials” is conceivable [18, 19]; these, however, found so far no chemical applications [19].

THE STRUCTURE-DEPENDENCE OF THE COEFFICIENTS OF THE CHARACTERISTIC AND PERMANENTAL POLYNOMIALS

The coefficients a_k of the characteristic polynomial can be computed from the structure of the graph G by means of the Sachs theorem [6]. The Sachs theorem is stated and exemplified in many books [1,3–5,20] and papers [21–26] and therefore we are repeating its necessary details as concise as possible.

A Sachs graph S is a graph in which all components are isolated edges and/or triangles and/or quadrangles and/or pentagons and/or hexagons Under “isolated edge” is meant a 2-vertex graph with one edge. Let $p(S)$ be the number of components of the Sachs graph S , and $c(S)$ the number of its cyclic components (triangles, quadrangles, . . .). Then the Sachs theorem reads:

$$a_k = \sum_S (-1)^{p(S)} 2^{c(S)} \quad (5)$$

with the summation running over all k -vertex Sachs graphs, that are as subgraphs contained in G .

Bearing in mind the definition of a permanent [8], for the coefficients of the permanental polynomial one has [9],

$$b_k = (-1)^k \sum_S (+1)^{p(S)} 2^{c(S)} = (-1)^k \sum_S 2^{c(S)}. \quad (6)$$

Equation (6) is a straightforward generalization of the Sachs formula. It is obtained from Eq. (3) in the very same way as formula (5) is obtained from Eq. (1). Formulas (5) and

(6) provide a general connection between the structure of a (molecular) graph and the coefficients of its characteristic and permanental polynomials, respectively.

Immediate consequences of (5) and (6) are:

$$a_0 = b_0 = 1 \quad ; \quad a_1 = b_1 = 0 \quad ; \quad -a_2 = b_2 = m \quad ; \quad a_3 = b_3 = -2c_3$$

where m is the number of edges and c_3 the number of triangles. From Eq. (6) it is also immediately seen that all even coefficients of $\pi(G)$ are positive (or zero), whereas all odd coefficients are negative (or zero). The signs of the coefficients of $\phi(G)$ follow, in the general case, a much more complicated pattern.

Consider now bipartite graphs (i. e., the molecular graphs of alternant hydrocarbons). These possess no odd-membered cycles. Consequently, all odd coefficients in both $\phi(G)$ and $\pi(G)$ are equal to zero. For bipartite graphs the even coefficients of $\phi(G)$ alternate in sign:

$$a_2 \leq 0 \quad ; \quad a_4 \geq 0 \quad ; \quad a_6 \leq 0 \quad ; \quad a_8 \geq 0 \quad ; \quad a_{10} \leq 0 \quad \dots$$

whereas, as already mentioned, the even coefficients of $\pi(G)$ are all positive (or zero).

RELATIONS BETWEEN THE COEFFICIENTS OF THE CHARACTERISTIC AND PERMANENTAL POLYNOMIALS OF BENZENOID HYDROCARBONS

In this section we assume that the graphs considered are bipartite. Needless to say that the molecular graphs of benzenoid hydrocarbons are bipartite. We say that a cycle contained in the graph G is a $(4t)$ -cycle if its size (= number of vertices) is equal to $4t$ for some integer t , and, therefore, divisible by 4. If sign is disregarded, then the first few coefficients of $\phi(G)$ coincide with the corresponding coefficients of $\pi(G)$. By comparing the right-hand sides of (5) and (6) we conclude that the equality $|a_{2k}| = b_{2k}$ will hold provided all $(2k)$ -vertex Sachs graphs (of the graph G) have either even or odd number of components. If, however, there are $(2k)$ -vertex Sachs graphs with both even and odd number of components, then $|a_{2k}| < b_{2k}$ because in formula (5) these will contribute with opposite signs (and thus subtract from each other) whereas in (6) they add. Such a situation happens if there is a $(2k)$ -vertex Sachs graph with a $(4t)$ -cycle (one component,

an odd number), because there are other $(2k)$ -vertex Sachs graphs which instead of that cycle have $2t$ isolated edges ($2t$ components, an even number). An example is depicted in Figure 1, where $t = 3$.

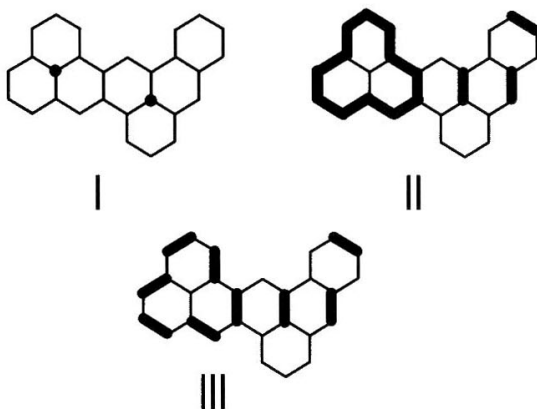


Figure 1. A pericondensed benzenoid system (I) with two inner vertices (marked by heavy dots); it has Sachs graphs containing a 12-membered cycle (e. g. II, $p = 4$, $c = 1$) as well as Sachs graphs in which instead of the 12-membered cycle there are 6 isolated edges (e. g. III, $p = 9$, $c = 0$); note that II has an even whereas III an odd number of components.

The smallest value of k for which the inequality $|a_{2k}| < b_{2k}$ will hold depends on the size of the shortest $(4t)$ -cycle in the graph G . Thus we arrive at:

Theorem 1. *Let G be a bipartite graph and q the size of its shortest $(4t)$ -cycle. Then for $k = 0, 1, \dots, q/2 - 1$,*

$$|a_{2k}| = b_{2k} \quad (7)$$

and $|a_q| < b_q$.

Corollary 1.1. *If G is acyclic, then Eq. (7) holds for all k .*

Corollary 1.2. *If G is a cyclic bipartite graph, but does not possess $(4t)$ -cycles, then Eq. (7) holds for all k .*

Catacondensed benzenoid systems do not possess $(4t)$ -cycles [27] and therefore, as a special case of Corollary 1.2 we have:

Corollary 1.3. *If G is the molecular graph of a catacondensed benzenoid hydrocarbon, then Eq. (7) holds for all k .*

Corollary 1.4. *Under the conditions specified in Theorem 1, $|a_q| = b_q - 4c_q$, where c_q is the number of q -membered cycles in G .*

An important special case of Corollary 1.4 is the below result for pericondensed benzenoid hydrocarbons. Note that these possess $(4t)$ -cycles. The shortest such cycles are 12-membered, a consequence of three hexagons sharing a common carbon atom, see [27] and cf. Figure 1. Therefore for pericondensed benzenoid systems, $q = 12$. Besides, c_q is just the number of internal vertices n_i , i. e., the number of vertices not belonging to the perimeter [27]. As discussed below, this special case applies rigorously only to planar benzenoid graphs; it does not necessarily apply, for example, to graphs of toroidal fullerenes.

Corollary 1.5. *If G is the molecular graph of a planar pericondensed benzenoid system with n_i internal vertices, then Eq. (7) is satisfied for $k = 0, 1, 2, 3, 4, 5$ whereas $|a_{12}| = b_{12} - 4n_i$.*

The above general results are, of course, in harmony with the examples communicated in

the paper [15]. Some additional calculations yielded the following:

In the case of phenalenyl, the monoradical $C_{13}H_9$, $b_k = |a_k|$ holds for all even coefficients, except for the last one. Since the perimeter of $C_{13}H_9$ is a 12-membered cycle, $b_{12} - |a_{12}| = 4$, as expected.

Triangulene, $C_{22}H_{12}$, which is a diradical, is a little more interesting. Here, $b_{12} - |a_{12}| = 16$ because there are 4 distinct 12-cycles. Furthermore, $b_{16} - |a_{16}| = 336 (= 84 \times 4)$ because it can be shown to derive from 9 distinct 16-membered cycles and 75 contributions from a 12-membered cycle plus two edges. Similarly, $b_{20} - |a_{20}| = 192 (= 48 \times 4)$ comes from 3 20-membered cycles, 30 sets of a 16-membered cycle plus 2 edges, and 15 sets of a 12-membered cycle plus 4 edges.

The most interesting aspect of these results is that it is the middle-sized cycles that make the largest contribution to $b_{20} - |a_{20}|$.

RELATIONS BETWEEN THE COEFFICIENTS OF THE CHARACTERISTIC AND PERMANENTAL POLYNOMIALS OF FULLERENES

The molecular graphs representing the carbon-atom skeleton of fullerenes are non-bipartite [28, 29]. They contain 12 pentagons (5-membered cycles). If these 12 pentagons are mutually disjoint then we say the respective fullerene obeys the “*isolated pentagon rule*” (*IPR*) or simply that it is an *IPR* fullerene [28, 29].

If two pentagons are not disjoint then they have an edge in common that is referred to as an 5,5-edge. Hence the number of 5,5-edges is equal to the number of pairs of non-disjoint pentagons. It is easy to envisage that each 5,5-edge implies the existence of an 8-membered cycle ($8 = 4t$, $t = 2$), see Figure 2. In view of this we denote the number of 5,5-edges by e_8 . Recall that in *IPR* fullerenes, $e_8 = 0$, and that otherwise $e_8 > 0$.

Using reasoning analogous to that leading to Theorem 1 we obtain:

Theorem 2. *Let G be a molecular graph of a fullerene in which $e_8 > 0$. Then for $k = 0, 1, \dots, 7$, $|a_k| = |b_k|$ and $|a_8| < b_8$.*

Corollary 2.1. *In the case of a fullerene specified in Theorem 2, $|a_8| = b_8 - 4e_8$ (cf.*

Corollary 1.4).

A noteworthy example of the relation given in Corollary 2.1 is found in the system C_{20} (the dodecahedron graph) studied in [15]. Here, calculation gave $b_8 = 10215$ and $a_8 = 10095 = b_8 - 4 \times 30$. In fact, C_{20} contains 30 8-membered cycles because all 30 of its edges separate two pentagons.

In non-bipartite graphs a new cause for the non-equality of $|a_{2k}|$ and b_{2k} may occur: It may happen that there is a $(2k)$ -vertex Sachs graph with a $(4t + 1)$ -cycle and another $(4t' + 1)$ -cycle (two components, an even number); in addition to it there will be other $(2k)$ -vertex Sachs graphs that instead of these cycles have $2t + 2t' + 1$ isolated edges ($2t + 2t' + 1$ components, an odd number). [The same situation is encountered with a Sachs graph possessing a $(4t + 3)$ -cycle and another $(4t' + 3)$ -cycle, but we will not pursue this (analogous, but chemically less interesting) case.]

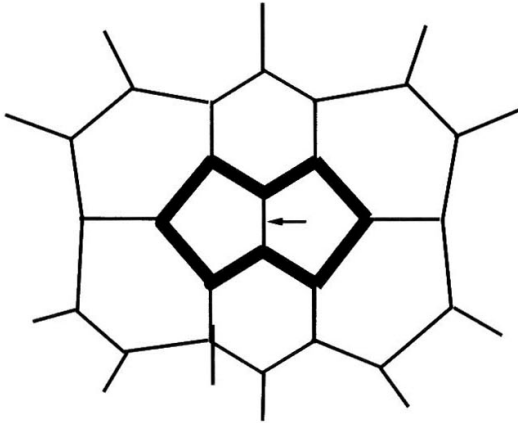


Figure 2. A detail of a fullerene skeleton in which two pentagons are not disjoint; the respective 5,5-edge is marked by an arrow and the 8-membered cycle induced by the two pentagons by heavy line.

Let us focus to *IPR* fullerenes. These do not contain 8-membered cycles. Their molecular graphs contain disjoint 5-membered cycles and therefore there exist Sachs graphs containing two 5-membered cycles ($t = t' = 1$). Then, instead of Theorem 2 we have:

Theorem 3. *Let G be a molecular graph of an *IPR* fullerene. Then for $k = 0, 1, \dots, 9$:*

$$|a_k| = |b_k| \quad (8)$$

and $|a_{10}| < b_{10}$.

Corollary 3.1. *If G is a molecular graph of an *IPR* fullerene, then, in addition to the relations (8), we have $|a_{10}| = b_{10} - 264$. Recall that $264 = 4 \binom{12}{2}$.*

The relations between the first few coefficients of $\phi(G)$ and $\pi(G)$ of fullerenes can be summarized as follows: For *IPR* fullerenes ($e_8 = 0$):

$$\begin{aligned} |a_k| &= |b_k| && \text{for } k = 1, 3, 5, 7, 9, 11, 13 \text{ and } k = 2, 4, 6, 8 \\ |a_k| &< |b_k| && \text{for } k = 15, 17, \dots \text{ and } k = 10, 12, \dots \end{aligned}$$

For fullerenes with 5,5-edges ($e_8 > 0$):

$$\begin{aligned} |a_k| &= |b_k| && \text{for } k = 1, 3, 5, 7, 9, 11 \text{ and } k = 2, 4, 6 \\ |a_k| &< |b_k| && \text{for } k = 13, 15, 17, \dots \text{ and } k = 8, 10, 12, \dots \end{aligned}$$

A NOTE ON 4-6 FULLERENES

In addition to “normal” fullerenes (in which the faces are pentagons or hexagons) chemical graph-theoreticians examined also 4-6 fullerenes (in which the faces are rectangles or hexagons) [30–33], and their boron–nitrogen analogs [34–36]. Indeed, the latter type seems to have actually been prepared [37].

According to Theorem 1, $|a_4| = b_4 - 4n_4$, where $n_4 = 6$, the number of quadrangles, and $|a_k| < b_k$ for $k = 6, 8, 10, \dots$. We have made a few observations about the polynomials of 4-6 fullerenes that, in our opinion, deserve to be mentioned here.

First of all, except for a few rare special cases, the rectangular faces must either be isolated (adjacent only to hexagons) or occur as 1, 2, or 3 pairs where each member of the pair

is adjacent to the other member of the pair and three hexagons. Thus, almost all 4-6 fullerenes have 0, 1, 2, or 3 pairs of adjacent rectangles. (The exceptions have either $4t$ vertices or $6t+2$ vertices for some integer t .) Now, it turns out that for n being the number of vertices, $b_8 - a_8$ is equal to $27n^2 - 378n + 1344$ regardless of the number of adjacent pairs. (The exceptions have a different value of $b_8 - a_8$ because they are tube-like structures that have 8-membered cycles around the circumference of the tube which do not include any edges of rectangular faces.) However, the individual values of b_8 and a_8 do depend on the number of adjacent pairs. Specifically, each adjacent pair has b_8 and a_8 larger by $3n - 26$ per adjacent pair than b_8 and a_8 for a structure with the same n and all isolated rectangles. Fitting the 7 data points we have available, it also turns out that b_8 (all isolated) is a 4th-order polynomial in n , namely, $b_8 = \frac{27}{128}n^4 - \frac{135}{32}n^3 + \frac{1401}{32}n^2 - \frac{2247}{8}n + 882$. For structures with adjacent pairs of rectangles, this is modified by adding $3n - 26$ per pair. Thus, we can at least say that the polynomial coefficients encode structural information about 4-6 fullerenes in a less than obvious way.

A NOTE ON ALL-HEXAGON, TOROIDAL FULLERENES

Euler's polyhedron closure rule demands that a polyhedron with all hexagonal faces be toroidal, i. e., that it have a surface of genus 1. Work on these structures was reviewed a few years ago [38]. Since that time, the permanent has been used to determine Kekulé structure counts [39], and actual samples have apparently been prepared and isolated [40]. Moreover, large-scale supercomputer simulations [41] have shown that all-hexagon forms are energetically more favorable than similar forms with topological (pentagon-heptagon) defects. Thus, the toroidal systems are chemically relevant.

Relationships between a_q and b_q that hold for planar benzenoids do not necessarily hold for toroidal benzenoids, at least not in the general case, since certain tube geometries allow cycles around the tube that cannot exist in planar systems. Kirby [38] has enumerated and described all the polyhex toroids through C_{60} , so all possible systems on ≤ 60 vertices can be examined individually. However, currently available computer resources limit the size of systems to 40 vertices. An immediately obvious difference between the toroidal and planar benzenoids is that all toroids on ≤ 40 vertices except one contain 8-membered

cycles. Surprisingly, the unique exception is not one of the 40-vertex systems, but a 38-vertex one, namely, the one designated 19-8-1 in Kirby's notation [38]. This structure has $|a_{12}| = b_{12} - 1292 = b_{12} - 4 \times 323$. Thus, each vertex participates, on average, in $323/38 = 8\frac{1}{2}$ 12-cycles. All the vertices are equivalent in the sense that they are all points where three hexagonal faces meet and no vertex need occupy any special place on the toroidal surface, so it might seem that the number of 12-cycles should be evenly divisible by the number of vertices. This is not the case because the vertex sites do not have the local threefold symmetry that internal vertices in a planar benzenoid graph have. In a planar benzenoid graph, all the 12-cycles are perimeters of a three-ring (phenalenyl) arrangement whose dual is a triangle. In the toroidal graph, on the other hand, some 12-cycles encircle the torus and are not the perimeter of any planar arrangement of hexagons. This effect should disappear when both the tube circumference and the internal torus circumference exceed 12 edges, but the Kirby *a-b-d* parameters for which this condition holds are not readily apparent.

From drawing the structures of the 7 possible 42-vertex all-hexagon toroids in parallelogram form [38], it appears that five among them contain 8-cycles, and the other two do not. It is not feasible with available equipment and algorithms, however, to compute the b_8 -values to confirm this. Assuming this finding is real, it would be interesting to investigate whether there is anything special about these two structures, and the unique one on 38 vertices, that distinguishes them from the other toroids of the same vertex counts, e. g., HOMO-LUMO gap, Kekulé structure count, strain energy, etc.

UNRESOLVED QUESTIONS

The work reported here suggests several questions about the systems considered (and others):

(1) With today's desktop computers, the characteristic polynomial for a system of any reasonable size can be found. The same cannot be said for the permanental polynomial. Can more efficient algorithms be developed so that permanental polynomials for larger systems can be studied?

(2) For the systems studied here, can profitable comparisons be made for a_k vs. b_k for larger k ?

(3) The present study treats only benzenoids and three types of fullerenes. For what other classes of polycyclic aromatic hydrocarbon graphs and cubic graphs might such comparisons yield unexpected structural information?

(4) What are the limiting toroidal tube diameter and internal torus diameter above which $|a_{12}| = b_{12} - 4n_i$, as it does for planar benzenoids? (For fullerenes, toroidal or otherwise, $4n_i$ is simply $4n$, since all the vertices are internal.) What relation, if any, exists between these diameters and the Kirby a - b - d notation for defining toroidal fullerene structures?

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