communications in mathematical
match
and in computer chemistry

no. 43, March 2001

ISSN 0340-6253

MATCDY (43) 49-66 (2001)

ON HOSOYA POLYNOMIALS OF BENZENOID GRAPHS

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(Received September 2000)

Abstract

For a connected graph G we denote by $d(G,k)$ the number of vertex pairs at distance k. Then the Hosoya polynomial of G is $H = \sum_{k\geq 0} d(G,k)\, x^k$. Some basic properties of the Hosoya polynomial of the molecular graphs of benzenoid molecules are established, and a recursive method for its calculation is presented. By means of this method explicit expressions for H are obtained for a number of homologous series of unbranched catacondensed benzenoid systems.

*Supported in part by the Ministry of Science and Technology of Slovenia under grant 101–504.
†Supported in part by the Ministry of Science and Technology of Slovenia under grant 101–511.

1. INTRODUCTION

In 1988 Hosoya [1] introduced a novel graphic polynomial $H(G,x)$ in the following manner. If G is a connected (molecular) graph with n vertices and m edges, and if $d(G,k)$ is the number of pairs of its vertices that are at distance k, then

$$H(G) \equiv H(G,x) = \sum_{k\geq 0} d(G,k)\, x^k \ .$$

Note that $d(G,0) = n$ and $d(G,1) = m$. For convenience we set $d(G,k) = 0$ for $k < 0$.

The main property of $H(G)$, that makes it interesting in chemistry, follows directly from its definition:

$$H'(G,1) = W(G) \tag{1}$$

where $H'(G,x)$ denotes the first derivative of $H(G,x)$ whereas $W(G)$ is the famous Wiener topological index (= the sum of distances between all pairs of vertices of G). Another elementary property of $H(G)$ is:

$$H(G,1) = \binom{n}{2} + n \ . \tag{2}$$

In view of Eq. (1) Hosoya named $H(G)$ the "*Wiener polynomial*". However, it is more justified and consistent with tradition to call it "*Hosoya polynomial*"; this name has been used in the recent papers on this matter [2]–[5]. It should be mentioned that the same graph polynomial was apparently independently conceived by Sagan et al. [6] who also called it "*Wiener polynomial*".

The hitherto published works on the Hosoya polynomial [1]–[10] report mainly results on trees, highly symmetric graphs and similar easy–to–handle objects. None of the papers [1]-[10] are concerned with polycyclic graphs, benzenoid systems in particular. This is in stark contrast to the work done on the Wiener index, where scores of publications dealing with benzenoid systems exist.

The aim of this paper is to contribute towards filling this gap. The definition of benzenoid graphs (molecular graphs representing benzenoid hydrocarbons) and a survey of their basic properties can be found in the book [11].

Concerning the chemical relevance and applications of the Hosoya polynomial we have, first of all, to point at the generalization of Eq. (1). Namely, if the first derivative of the Hosoya polynomial evaluated at x=1 is a useful topological index (the Wiener index), then also the "extended Wiener indices": the second, third, etc. derivatives of the same polynomial evaluated at x=1, may be of some chemical applicability. This fact was first demonstrated by Estrada et al. [12] and recently also by Konstantinova and Diudea [13]. In both works various physico-chemical properties of alkanes were shown to be well reproduced by means of linear combinations of the extended Wiener indices.

The Hosoya polynomial contains more information on the distance-relations in a (molecular) graph than any of the hitherto proposed distance-based topological indices. In view of this it imaginable that the Hosoya polynomial and the quantities derived from it will play a significant role in QSPR and QSAR studies. The demonstration of this, in spite of the preliminary success achieved in [12, 13], remains a task for the future.

2. HOSOYA POLYNOMIALS OF BENZENOID GRAPHS – SOME ELEMENTARY RESULTS

We start this section with two examples, the benzenoid graphs G_1 and G_2 (pertaining to anthracene and phenanthrene, respectively), depicted in Fig. 1.

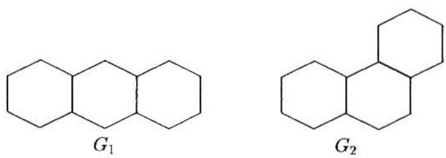

Figure 1: Two benzenoid graphs

It is easy to check that

$$H(G_1, x) = 14 + 16x + 22x^2 + 21x^3 + 14x^4 + 10x^5 + 6x^6 + 2x^7 \quad \text{and}$$
$$H(G_2, x) = 14 + 16x + 22x^2 + 22x^3 + 16x^4 + 10x^5 + 4x^6 + x^7 \, .$$

Note that neither the coefficients of $H(G_1)$ dominate those of $H(G_2)$ nor vice versa. However, the equality $d(G_1, 2) = d(G_2, 2)$ is no coincidence. From the first part of the next result it follows that this happens for all catacondensed benzenoid graphs with equal number of hexagons.

Proposition 1. Let G be a benzenoid graph with h hexagons, n_i internal vertices and b bay regions [11]. Further, let d be the number of pairs of adjacent hexagons of G. Then

(i) $d(G, 2) = 8h - 2 - n_i$;
(ii) $d(G, 3) = 3h + 6d + b$.

Proof. (i) In triangle–free graphs (such as the benzenoid graphs) two vertices are at distance 2 if they have a common neighbor. The number of vertex pairs having vertex i as a common neighbor is $\binom{\delta_i}{2}$, where δ_i is the degree of the vertex i. Benzenoid graphs have only vertices of degree two and three. Thus

$$d(G, 2) = \sum_{i=1}^{n} \binom{\delta_i}{2} = n_2 \binom{2}{2} + n_3 \binom{3}{2} = n_2 + 3\, n_3$$

where n_2 and n_3 are the numbers of vertices of degree 2 and 3, respectively. It is known that [11]

$$n_3 = 2(h - 1) \qquad ; \qquad n_2 = 2h + 4 - n_i$$

from which formula (i) follows directly.

(ii) Note first that in every hexagon there are 3 pairs of vertices at distance 3. In addition, for each pair of adjacent hexagons there are precisely 6 pairs of vertices (not belonging to the same hexagon) at distance 3. Moreover, the only possibility for two vertices being at distance 3 and not lying in the same hexagon or in adjacent hexagons is that they belong to a bay. Since each bay corresponds to exactly one such pair we are done. □

We wish to add that the number d from the above proposition is also equal to the number of 10-cycles of G, i.e., the number of naphthalene units. Also note that the second part of the Proposition 1 implies that $d(G,3)$ is minimal (among catacondensed benzenoid graph with h hexagons) for linear polyacenes with h hexagons.

For a graph G, $k \geq 0$, and a vertex $v \in V(G)$, let $d(G,v,k)$ be the number of vertices of G at distance k from v. This time, $d(G,v,0) = 1$, and for $k < 0$ we set $d(G,v,k) = 0$. We now define $H(G,v,x)$ as

$$H(G,v) \equiv H(G,v,x) = \sum_{k \geq 0} d(G,v,k)x^k .$$

With this definition, we have the following easy identity.

Proposition 2. For any graph G,

$$\sum_{v \in V(G)} H(G,v,x) = 2\,H(G,x) - |V(G)| .$$

Proof. Just observe that

$$\sum_{v \in V(G)} d(G,v,k) = \begin{cases} d(G,k) & \text{if} \quad k = 0, \\ 2d(G,k) & \text{if} \quad k > 0. \end{cases} \qquad \square$$

3. ANNELATING 6–CYCLES

We are interested in graphs that can be recursively constructed from smaller ones by attaching cycles. In graph theory such an operation is usually called "*amalgamation*" of (two) graphs over a common subgraph. In our case, the common subgraph will always be an edge, and one of the amalgamated graphs will be a 6-cycle, cf. Fig. 2. In chemistry "amalgamation of a cycle" is referred to as "*annelation*".

Proposition 3. Let the graph G be obtained by annelating a 6-cycle to the graph G_0 over an edge uv. Then

$$\begin{aligned} H(G,x) &= H(G_0,x) + (x+x^2)H(G_0,u,x) + (x+x^2)H(G_0,v,x) \\ &+ 4 + 3x + 2x^2 + x^3 . \end{aligned}$$

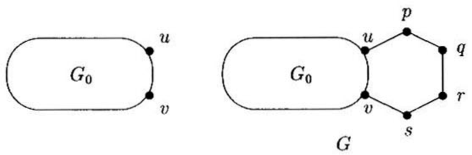

Figure 2: G is obtained by annelating a 6-cycle to G_0 over the edge uv

Proof. We first write the Hosoya polynomial of G as:

$$H(G,x) = d(G,0) + d(G,1)x + d(G,2)x^2 + d(G,3)x^3 + \sum_{k\geq 4} d(G,k)x^k\ . \qquad (3)$$

Denoting the expression

$$d(G_0,k) + d(G_0,u,k-1) + d(G_0,u,k-2) + d(G_0,v,k-1) + d(G_0,v,k-2)$$

by $d(G_0,k,u,v)$ we infer that

$$d(G,k) = \begin{cases} d(G_0,k,u,v) & \text{if} \quad k > 3\ , \\ d(G_0,k,u,v)+1 & \text{if} \quad k = 3\ , \\ d(G_0,k,u,v)+2 & \text{if} \quad k = 2\ , \\ d(G_0,k,u,v)+3 & \text{if} \quad k = 1\ , \\ d(G_0,k,u,v)+4 & \text{if} \quad k = 0\ . \end{cases}$$

Inserting this into (3) we find that $H(G,x)$ can be expressed as

$$\sum_{k\geq 0} d(G_0,k,u,v)x^k + 4 + 3x + 2x^2 + x^3\ ,$$

which, in turn, is equal to

$$H(G_0,x) + xH(G_0,u,x) + x^2H(G_0,u,x) + xH(G_0,v,x) + x^2H(G_0,v,x)$$
$$+ 4 + 3x + 2x^2 + x^3\ . \quad \square$$

Let G be obtained by annelating a 6-cycle to G_0 and let the vertices of this 6-cycle be labeled by u, v, s, r, q, and p, as indicated in Fig. 2. In order to compute $H(G,x)$ we also need to express $H(G,p,x)$, $H(G,s,x)$, $H(G,q,x)$, and $H(G,r,x)$ recursively. This is achieved in the following:

Proposition 4. Let G, G_0, u, v, s, r, q, and p be as in Fig. 2. Then

(i) $H(G,p,x) = xH(G_0,u,x) + 1 + x + x^2 + x^3$,

(ii) $H(G,s,x) = xH(G_0,v,x) + 1 + x + x^2 + x^3$,

(iii) $H(G,q,x) = x^2H(G_0,u,x) + 1 + 2x + x^2$,

(iv) $H(G,r,x) = x^2H(G_0,v,x) + 1 + 2x + x^2$.

Proof. By symmetry it is sufficient to prove (i) and (iii). For (i) note first that

$$d(G,p,k) = \begin{cases} d(G_0,u,k-1) & \text{if} \quad k > 3 \ , \\ d(G_0,u,k-1)+1 & \text{if} \quad 0 \le k \le 3 \ . \end{cases}$$

Then we have

$$\begin{aligned} H(G,p,x) &= \sum_{k\geq 0} d(G,p,k)x^k \\ &= \sum_{k\geq 0} d(G_0,u,k-1)x^k + 1 + x + x^2 + x^3 \\ &= xH(G_0,u,x) + 1 + x + x^2 + x^3 \ . \end{aligned}$$

Similarly, in order to obtain recursion (iii) we first observe that

$$d(G,q,k) = \begin{cases} d(G_0,u,k-2) & \text{if} \quad k > 2 \ , \\ d(G_0,u,k-2)+1 & \text{if} \quad k = 2 \ , \\ d(G_0,u,k-2)+2 & \text{if} \quad k = 1 \ , \\ d(G_0,u,k-2)+1 & \text{if} \quad k = 0 \ , \end{cases}$$

from which we conclude that

$$\begin{aligned} H(G,q,x) &= \sum_{k\geq 0} d(G,q,k)x^k \\ &= \sum_{k\geq 0} d(G_0,u,k-2)x^k + 1 + 2x + x^2 \\ &= x^2H(G_0,u,x) + 1 + 2x + x^2 \ . \quad \square \end{aligned}$$

At this point it should be mentioned that the results presented here as Propositions 3 and 4 are fully analogous to the formulas earlier obtained for the Wiener index [14]. In fact, these earlier results can be deduced, as special cases, from Propositions 3 and 4, by computing the first derivatives of the respective polynomials, by setting $x = 1$ and by using Eqs. (1) and (2). In a similar manner, the applications of the Propositions 3 and 4, outlined in the subsequent section, can be viewed as generalizations of the results for the Wiener index, communicated in [15].

4. APPLICATION TO HEXAGONAL CHAINS

We now apply the previous recursive relations to hexagonal chains. Let B_h be a hexagonal chain with h hexagons obtained by adding a 6-cycle to B_{h-1} over an edge $u_{h-1}v_{h-1}$. Then by Proposition 3 we have

$$\begin{aligned} H(B_h,x) &= H(B_{h-1},x) + (x+x^2)\Big[H(B_{h-1},u_{h-1},x) + H(B_{h-1},v_{h-1},x)\Big] \\ &\quad + 4 + 3x + 2x^2 + x^3\,. \end{aligned}$$

Furthermore, let $u_h v_h$ be the edge that will be used in the subsequent annelation, that is, in the process $B_h \to B_{h+1}$. There are three possibilities for the edge $u_h v_h$ and these are shown in Fig. 3.

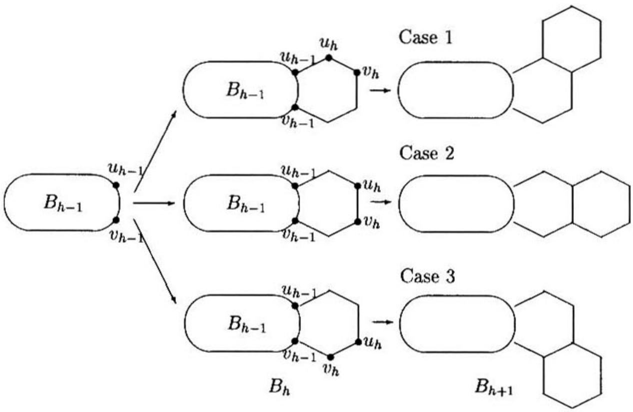

Figure 3: Three possible ways of attaching a 6-cycle to a hexagonal chain

For these three cases Proposition 4 implies:

Case 1:

$$H(B_h, u_h, x) = xH(B_{h-1}, u_{h-1}, x) + 1 + x + x^2 + x^3 ,$$
$$H(B_h, v_h, x) = x^2 H(B_{h-1}, u_{h-1}, x) + 1 + 2x + x^2.$$

Case 2:

$$H(B_h, u_h, x) = x^2 H(B_{h-1}, u_{h-1}, x) + 1 + 2x + x^2 ,$$
$$H(B_h, v_h, x) = x^2 H(B_{h-1}, v_{h-1}, x) + 1 + 2x + x^2.$$

Case 3:

$$H(B_h, u_h, x) = x^2 H(B_{h-1}, v_{h-1}, x) + 1 + 2x + x^2 ,$$
$$H(B_h, v_h, x) = xH(B_{h-1}, v_{h-1}, x) + 1 + x + x^2 + x^3.$$

We write the above recurrences in a more concise form by setting $\alpha_h \equiv H(B_h, x)$, $\beta_h \equiv H(B_h, u_h, x)$, and $\gamma_h \equiv H(B_h, v_h, x)$. Then we have:

Proposition 5. Let B_h be a hexagonal chain with h hexagons. Then the Hosoya polynomial α_h of B_h satisfies the following recurrence

$$\alpha_h = \alpha_{h-1} + (x + x^2)(\beta_{h-1} + \gamma_{h-1}) + 4 + 3x + 2x^2 + x^3 ,$$

where $\alpha_0 = 2 + x$, $\beta_0 = \gamma_0 = 1 + x$. Moreover, β_h and γ_h obey the following recurrences, depending on the cases shown in Fig. 3:

Case 1: $\beta_h = x\beta_{h-1} + 1 + x + x^2 + x^3$; $\gamma_h = x^2\beta_{h-1} + 1 + 2x + x^2$.

Case 2: $\beta_h = x^2\beta_{h-1} + 1 + 2x + x^2$; $\gamma_h = x^2\gamma_{h-1} + 1 + 2x + x^2$.

Case 3: $\beta_h = x^2\gamma_{h-1} + 1 + 2x + x^2$; $\gamma_h = x\gamma_{h-1} + 1 + x + x^2 + x^3$.

5. HOSOYA POLYNOMIALS OF PERIODIC HEXAGONAL CHAINS

A hexagonal chain B_n consisting of $n \geq 1$ hexagons corresponds to a walk of length $n-1$ on the inner dual of the respective chain, where each next step is either straight, a 60-degree turn to the left, or a 60-degree turn to the right (relatively to the previous step). We encode such a walk by a string of length n over the alphabet $\{1,2,3\}$ where 1, 2, and 3 mean "turn left", "go straight", and "turn right", respectively. The first and the last symbol of this string are immaterial – they are included in order for this encoding scheme to cover all B_n with $n \geq 0$. For example, B_0 is encoded by the empty string, B_1 by any string of length one, and B_2 by any string of length two. The graphs G_1 and G_2 of Fig. 1 are encoded by $x2y$ and $x1y$, respectively, where x and y are arbitrary elements of $\{1,2,3\}$.

Take any nonempty finite string s over $\{1,2,3\}$, and repeat it infinitely often to obtain the infinite string $S = sss\ldots$. Let B_n denote the hexagonal chain corresponding to the initial substring of S of length n, and let $H(B_n,x)$ denote its Hosoya polynomial. From Proposition 5 it follows that the sequence of polynomials $H(B_n,x)$, together with the corresponding sequences β_n and γ_n, satisfies a system of linear recurrences with constant coefficients, where the structure of each individual recurrence depends on the remainder of n modulo the length of s. Such sequences are said to be *conditional recurrent* and are known to satisfy a single (unconditional) linear recurrence with constant coefficients (cf. [16]). Therefore $H(B_n,x)$ are exponential polynomials in n (i.e., $H(B_n,x)$ has the form $\sum_{k=0}^{m} P_k(n)c_k^n$ where $P_k(n)$ are polynomials in n with coefficients that are rational functions of x, and c_k's are rational functions of x which are independent of n), and their generating function

$$f(x,z) = \sum_{n=0}^{\infty} H(B_n,x)z^n$$

is a rational function of z and x. It can be computed as follows: Let d denote the length of s, and let $\beta_n^{(k)} = \beta_{dn+k}$ and $\gamma_n^{(k)} = \gamma_{dn+k}$, for $0 \leq k \leq d-1$. Then we have the following system of $2d$ initial conditions

$$\begin{aligned} \beta_0^{(0)} &= \gamma_0^{(0)} = 1 + x, \\ \beta_0^{(k)} &= \gamma_0^{(k)} = 0 \quad (1 \leq k \leq d-1) \end{aligned}$$

and $2d$ (unconditional, as far as n is concerned) recurrences

$$\beta_n^{(0)} = \begin{cases} x\beta_{n-1}^{(d)} + p, & s_1 = 1 \\ x^2\beta_{n-1}^{(d)} + q, & s_1 = 2 \\ x^2\gamma_{n-1}^{(d)} + q, & s_1 = 3, \end{cases}$$

$$\beta_n^{(k)} = \begin{cases} x\beta_n^{(k-1)} + p, & s_{k+1} = 1 \\ x^2\beta_n^{(k-1)} + q, & s_{k+1} = 2 \\ x^2\gamma_n^{(k-1)} + q, & s_{k+1} = 3 \end{cases} \qquad (1 \le k \le d-1),$$

$$\gamma_n^{(0)} = \begin{cases} x^2\beta_{n-1}^{(d)} + q, & s_1 = 1 \\ x^2\gamma_{n-1}^{(d)} + q, & s_1 = 2 \\ x\gamma_{n-1}^{(d)} + p, & s_1 = 3, \end{cases}$$

$$\gamma_n^{(k)} = \begin{cases} x^2\beta_n^{(k-1)} + q, & s_{k+1} = 1 \\ x^2\gamma_n^{(k-1)} + q, & s_{k+1} = 2 \\ x\gamma_n^{(k-1)} + p, & s_{k+1} = 3 \end{cases} \qquad (1 \le k \le d-1),$$

where $p = 1 + x + x^2 + x^3$, $q = (1+x)^2$, and s_k denotes the k-th symbol of s. Given the string s, one can routinely compute from this system the generating functions of $\beta_n^{(k)}$ and $\gamma_n^{(k)}$. These can easily be combined to yield the generating functions of their interlacings β_n and γ_n, from which we finally compute the desired generating function $f(x,z)$ of $\alpha_n = H(B_n, x)$.

We wrote a *Mathematica* package[1] (based on the standard package `RSolve.m`) which, given a nonempty string s over $\{1,2,3\}$, in the way just described, computes the corresponding rational generating function $f(x,z)$, and (if the denominator of $f(x,z)$ factors nicely, which unfortunately is not necessarily the case) also the formula giving the n-th Hosoya polynomial $H(B_n, x)$ as a function of n. It seems however, that for the class of problems studied here the denominator of

$$f(x,z,k) = \sum_{n=0}^{\infty} H(B_{dn+k}, x) z^n$$

where d is the length of s and $0 \le k < d$, does always factor nicely. If so, then our package can always compute the d formulas giving $H(B_{dn+k}, x)$ as functions of n, for $0 \le k < d$. It can also compute the corresponding Wiener indices $W(B_n) = H'(B_n, 1)$ and $W(B_{dn+k}) = H'(B_{dn+k}, 1)$ as functions of n, for $0 \le k < d$.

In the rest of this section we list the formulas (obtained by our package) for $f(x,z)$, and either $H(B_n,x)$ and $W(B_n)$, or $H(B_{dn+k},x)$ and $W(B_{dn+k})$, for various strings s encoding periodic hexagonal chains as described in Section 5. Even though $H(B_n,x)$ appear to be rational or even algebraic functions of x, they simplify to a polynomial in x for each specific value of n. The formulas that follow are valid for all $n \ge 0$, unless stated otherwise.

[1] available at `http://www.fmf.uni-lj.si/~petkovsek/software.html` in the notebook `Hosoya.nb`

The straight-line chain: $s = 2$

$$f(x,z) = \frac{(x^5 - 2x^3)\,z^2 + (-2x^3 - 4x^2 - 4x - 2)\,z - x - 2}{(z-1)^2\,(x^2 z - 1)}$$

$$H(B_n,x) = \frac{2\,(x+1)\,x^{2n+2} - x^3 - 2x^2 - 3x + n\,(x-1)\,(x^2+1)\,(x^2 - x - 4) + 2}{(x-1)^2}$$

$$W(B_n) = \frac{1}{3}\,(16\,n^3 + 36\,n^2 + 26\,n + 3)$$

The spiral chain: $s = 1$

$$f(x,z) = \frac{1}{(z-1)^2\,(x\,z-1)}((-x^7 - 2x^6 + 2x^4 + x^3)\,z^3 + (-2x^5 - 3x^4 + 2x^2 + 2x)\,z^2 + (-3x^3 - 5x^2 - 2x - 2)\,z - x - 2)$$

$n \geq 1$:

$$H(B_n,x) = \frac{1}{(x-1)^2}((x+1)^4\,x^{n+2} + x^8 - 4x^6 - 4x^5 - 3x^4 - 3x^3 - 2x^2 - 3x - n\,(x-1)\,(x^2+1)\,(x^5 + 2x^4 + x^3 - x^2 + x + 4) + 2)$$

$$n \geq 1: \quad W(B_n) = \frac{1}{3}\,(8\,n^3 + 72\,n^2 - 26\,n + 27)$$

The zig-zag chain: $s = 13$

$$f(x,z) = \frac{(x^7 + 2x^6 - 2x^4 - x^3)\,z^3 + (x^5 - 2x^3)\,z^2 + (-2x^3 - 4x^2 - 4x - 2)\,z - x - 2}{(z-1)^2\,(x^2 z - 1)}$$

$$n \geq 1: \quad H(B_n,x) = \frac{1}{(x-1)^2}((x+1)^2\,x^{2n+1} - x^7 + 3x^5 - 3x^3 - 2x^2 - 3x + n\,(x-1)\,(x^6 + x^5 - 2x^3 - 3x^2 - x - 4) + 2)$$

$$n \geq 1: \quad W(B_n) = \frac{1}{3}\,(16\,n^3 + 24\,n^2 + 62\,n - 21)$$

The double-step zig-zag: $s = 2123$

$$f(x,z) = ((x^9 + 2\,x^8 - 2\,x^6 - x^5)\,z^5 + (x^7 + 2\,x^6 + x^5 - 2\,x^4 - 3\,x^3)\,z^3 + (x^5 - 4\,x^3 - 4\,x^2 - 4\,x - 2)\,z^2 + (-2\,x^3 - 4\,x^2 - 5\,x - 4)\,z - x - 2)/ ((z-1)^2\,(z+1)\,(x^2\,z - 1))$$

$n \geq 2$:

$$H(B_n, x) = \frac{1}{4\,(x-1)^2}(4\,(x+1)^2\,x^{2\,n+1} - 5\,x^9 + 11\,x^7 - 3\,x^5 + (-1)^n\,(x-1)^3\,(x+1)^3\,x^3 - 7\,x^3 - 8\,x^2 - 12\,x + 2\,n\,(x-1)\,(x^2-2)\,(x^2+1)\,(x^4 + x^3 + x^2 + x + 4) + 8)$$

$$n \geq 2: \quad W(B_n) = \frac{1}{3}\,(16\,n^3 + 24\,n^2 + 74\,n + 6\,(-1)^n - 51)$$

The triple-step zig-zag: $s = 221223$

$$f(x,z) = ((x^{11} + 2\,x^{10} - 2\,x^8 - x^7)\,z^7 + (x^9 + 2\,x^8 + x^7 - 2\,x^4 - 3\,x^3)\,z^4 + (x^5 - 4\,x^3 - 4\,x^2 - 4\,x - 2)\,z^3 + (x^5 - 4\,x^3 - 4\,x^2 - 5\,x - 4)\,z^2 + (-2\,x^3 - 4\,x^2 - 5\,x - 4)\,z - x - 2)/ ((z-1)^2\,(x^2\,z-1)\,(z^2+z+1))$$

$n \geq 1$:

$$H(B_{6n}, x) = \frac{1}{(x-1)^2}((x+1)^2\,x^{12\,n+1} - x^{11} + 2\,x^9 - x^7 + x^5 - 2\,x^3 - 2\,x^2 - 3\,x + 2\,n\,(x-1)\,(x^{10} + x^9 + 2\,x^4 - 4\,x^3 - 9\,x^2 - 3\,x - 12) + 2)$$

$n \geq 1$:

$$H(B_{6n+1}, x) = \frac{1}{(x-1)^2}((x+1)^2\,x^{12\,n+3} - x^{11} + 2\,x^9 - 2\,x^4 - 3\,x^3 - 6\,x + 2\,n\,(x-1)\,(x^{10} + x^9 + 2\,x^4 - 4\,x^3 - 9\,x^2 - 3\,x - 12) + 6)$$

$n \geq 1$:

$$H(B_{6n+2}, x) = \frac{1}{(x-1)^2}((x+1)^2\,x^{12\,n+5} - x^{11} + 3\,x^9 - 2\,x^7 + 2\,x^5 - 4\,x^4 - 5\,x^3 + 2\,x^2 - 9\,x + 2\,n\,(x-1)\,(x^{10} + x^9 + 2\,x^4 - 4\,x^3 - 9\,x^2 - 3\,x - 12) + 10)$$

$$H(B_{6n+3}, x) = \frac{1}{(x-1)^2}((x+1)^2\,x^{12\,n+7} + x^9 - x^7 + 3\,x^5 - 6\,x^4 - 7\,x^3 + 4\,x^2 - 12\,x + 2\,n\,(x-1)\,(x^{10} + x^9 + 2\,x^4 - 4\,x^3 - 9\,x^2 - 3\,x - 12) + 14)$$

$$H(B_{6n+4},x) = \frac{1}{(x-1)^2}((x+1)^2\,x^{12\,n+9} + x^9 + 2\,x^5 - 8\,x^4 - 8\,x^3 + 6\,x^2 - 15\,x + 2\,n\,(x-1)\,(x^{10} + x^9 + 2\,x^4 - 4\,x^3 - 9\,x^2 - 3\,x - 12) + 18)$$

$$H(B_{6n+5},x) = \frac{1}{(x-1)^2}((x+1)^2\,x^{12n+11} + 2\,(x^9 - x^7 + 2\,x^5 - 5\,x^4 - 5\,x^3 + 4\,x^2 - 9\,x + 11) + 2\,n\,(x-1)\,(x^{10} + x^9 + 2\,x^4 - 4\,x^3 - 9\,x^2 - 3\,x - 12))$$

$$n \geq 1: \quad W(B_{6n}) = 1152\,n^3 + 288\,n^2 + 172\,n - 23$$

$$n \geq 1: \quad W(B_{6n+1}) = 1152\,n^3 + 864\,n^2 + 364\,n + 11$$

$$n \geq 1: \quad W(B_{6n+2}) = 1152\,n^3 + 1440\,n^2 + 748\,n + 101$$

$$W(B_{6n+3}) = 1152\,n^3 + 2016\,n^2 + 1324\,n + 279$$

$$W(B_{6n+4}) = 1152\,n^3 + 2592\,n^2 + 2092\,n + 553$$

$$W(B_{6n+5}) = 1152\,n^3 + 3168\,n^2 + 3052\,n + 979$$

The double-step spiral: $s = 21$

$$f(x,z) = ((-x^{11} - 2\,x^{10} + 2\,x^8 + x^7)\,z^6 + (-x^9 - 2\,x^8 + 2\,x^6 + x^5)\,z^5 + (-x^9 - 2\,x^8 - 2\,x^7 - x^6 + x^5 + 2\,x^4 + 2\,x^3)\,z^4 + (-x^7 - x^6 - 2\,x^5 - 5\,x^4 - 3\,x^3 - 2\,x^2)\,z^3 + (-2\,x^5 - 5\,x^4 - 7\,x^3 - 8\,x^2 - 4\,x - 2)\,z^2 + (-3\,x^3 - 6\,x^2 - 5\,x - 4)\,z - x - 2)/((z-1)^2\,(z+1)\,(x^3\,z^2 - 1))$$

$n \geq 2$:

$$H(B_n,x) = (2\,(x+1)^5\,(x^2 + x^{3/2} + \sqrt{x} + 1 + (-1)^n\,(x^2 - x^{3/2} - \sqrt{x} + 1))\,x^{\frac{3n}{2}+2} + 5\,x^{14} + 10\,x^{13} + 4\,x^{12} - 11\,x^{11} - 22\,x^{10} - 18\,x^9 - 18\,x^8 - 26\,x^7 - 35\,x^6 - 52\,x^5 - 54\,x^4 - (-1)^n\,(x-1)^2\,(x+1)^3\,(x^2 + x + 1)\,(x^4+1)\,x^3 - 43\,x^3 - 8\,x^2 + 4\,x - 2\,n\,(x-1)\,(x^2+1)\,(x^2 + x + 1)\,(x^9 + 2\,x^8 + x^7 + x^5 + x^3 + 8\,x^2 + 10\,x + 8) + 8)/(4\,(x-1)^2\,(x^2+x+1)^2)$$

$$n \geq 2: \quad W(B_n) = 4\,n^3 + 20\,n^2 - 12\,n + 2\,(-1)^n\,(n-2) + 21$$

The triple-step spiral: $s = 221$

$$f(x,z) = ((-x^{15} - 2x^{14} + 2x^{12} + x^{11})z^9 + (-x^{13} - 2x^{12} + 2x^{10} + x^9)z^8 + (-x^{11} - 2x^{10} + 2x^8 + x^7)z^7 + (-x^{13} - 2x^{12} - x^{11} - x^9 - x^8 + x^7 + 2x^6 + 2x^5)z^6 + (-x^{11} - 2x^{10} - x^9 + x^8 - x^7 - 5x^6 - 3x^5 - 2x^4)z^5 + (-x^9 - x^8 - x^7 - 3x^6 - 5x^5 - 10x^4 - 7x^3 - 2x^2)z^4 + (-2x^7 - 5x^6 - 6x^5 - 8x^4 - 9x^3 - 8x^2 - 4x - 2)z^3 + (-2x^5 - 6x^4 - 9x^3 - 8x^2 - 5x - 4)z^2 + (-3x^3 - 6x^2 - 5x - 4)z - x - 2)/((z-1)^2(z^2+z+1)(x^5z^3-1))$$

$n \geq 1$:

$$H(B_{3n},x) = ((x+1)^4(x^2-x+1)(x^2+x+1)(x^3+x+1)x^{5n+2} + x^{20} + 2x^{19} + x^{18} - 2x^{15} - 5x^{14} - 5x^{13} - 5x^{12} - 7x^{11} - 10x^{10} - 15x^9 - 18x^8 - 21x^7 - 22x^6 - 20x^5 - 12x^4 - 7x^3 - 2x^2 + x - n(x-1)(x^2+1)(x^4+x^3+x^2+x+1)(x^{13} + 2x^{12} + x^{11} + x^9 + 2x^8 + x^7 - 3x^6 + x^5 + 14x^4 + 13x^3 + 12x^2 + 15x + 12) + 2)/((x-1)^2(x^4+x^3+x^2+x+1)^2)$$

$n \geq 1$:

$$H(B_{3n+1},x) = ((x+1)^4(x^3+x+1)(x^3+x^2+1)x^{5n+4} + x^{20} + 2x^{19} + x^{18} - x^{16} - 4x^{15} - 6x^{14} - 4x^{13} - 5x^{12} - 9x^{11} - 13x^{10} - 24x^9 - 29x^8 - 29x^7 - 24x^6 - 19x^5 - 2x^4 + 3x^3 + 6x^2 + 6x - n(x-1)(x^2+1)(x^4+x^3+x^2+x+1)(x^{13} + 2x^{12} + x^{11} + x^9 + 2x^8 + x^7 - 3x^6 + x^5 + 14x^4 + 13x^3 + 12x^2 + 15x + 12) + 6)/((x-1)^2(x^4+x^3+x^2+x+1)^2)$$

$n \geq 1$:

$$H(B_{3n+2},x) = ((x+1)^4(x^3+x+1)^2x^{5n+6} + x^{20} + 2x^{19} - 2x^{17} - 2x^{16} - 4x^{15} - 6x^{14} - 2x^{13} - 4x^{12} - 13x^{11} - 18x^{10} - 32x^9 - 39x^8 - 36x^7 - 24x^6 - 18x^5 + 6x^4 + 12x^3 + 14x^2 + 11x - n(x-1)(x^2+1)(x^4+x^3+x^2+x+1)(x^{13} + 2x^{12} + x^{11} + x^9 + 2x^8 + x^7 - 3x^6 + x^5 + 14x^4 + 13x^3 + 12x^2 + 15x + 12) + 10)/((x-1)^2(x^4+x^3+x^2+x+1)^2)$$

$n \geq 1: \quad W(B_{3n}) = 120n^3 + 168n^2 - 34n + 25$

$n \geq 1: \quad W(B_{3n+1}) = 120n^3 + 288n^2 + 102n + 43$

$n \geq 1: \quad W(B_{3n+2}) = 120n^3 + 408n^2 + 334n + 117$

$s = 1133$

$$f(x,z) = ((x^8 + 2x^7 - 2x^5 - x^4)\,z^5 + (-x^9 - 2x^8 - x^7 + x^6 + x^5 + x^3)\,z^4 +$$
$$(-x^7 - x^6 - 2x^5 - 5x^4 - 3x^3 - 2x^2)\,z^3 +$$
$$(-2x^5 - 5x^4 - 7x^3 - 8x^2 - 4x - 2)\,z^2 +$$
$$(-3x^3 - 6x^2 - 5x - 4)\,z - x - 2)/((z-1)^2\,(z+1)\,(x^3 z^2 - 1))$$

$n \geq 1:$

$$H(B_n, x) = (2\,(x+1)^4\,(x^2+1)\,(x^2 + x^{3/2} + \sqrt{x} + 1 + (-1)^n\,(x^2 - x^{3/2} -$$
$$\sqrt{x} + 1))\,x^{\frac{3n}{2}+1} + x^{12} - x^{11} - 6x^{10} - 7x^9 - 6x^8 - 11x^7 - 38x^6 -$$
$$73x^5 - (-1)^n\,(x-1)^2\,(x+1)^4\,(x^2+x+1)\,x^4 - 71x^4 - 48x^3 - 8x^2 +$$
$$4x - 2n\,(x-1)\,(x^2+x+1)\,(x^9 + x^8 + 5x^5 + 11x^4 + 12x^3 + 16x^2 +$$
$$10x + 8) + 8)/(4\,(x-1)^2\,(x^2+x+1)^2)$$

$$n \geq 1: \quad W(B_n) = 4n^3 + 16n^2 + 8n + 2\,(-1)^n\,(n-2) - 3$$

$s = 111333$

$$f(x,z) = ((x^9 + 2x^8 - 2x^6 - x^5)\,z^7 + (-x^{10} - 2x^9 - x^8 + x^7 + x^6 + x^4)\,z^6 +$$
$$(-x^{10} - 3x^9 - 4x^8 - 2x^7 - x^6 - 2x^5 - x^3)\,z^5 +$$
$$(-x^8 - 2x^7 - 4x^6 - 7x^5 - 7x^4 - 7x^3 - 2x^2)\,z^4 +$$
$$(-x^7 - 4x^6 - 7x^5 - 8x^4 - 10x^3 - 8x^2 - 4x - 2)\,z^3 +$$
$$(-2x^5 - 6x^4 - 9x^3 - 8x^2 - 5x - 4)\,z^2 +$$
$$(-3x^3 - 6x^2 - 5x - 4)\,z - x - 2)/((z-1)^2\,(z^2+z+1)\,(x^4 z^3 - 1))$$

$n \geq 1:$

$$H(B_{6n}, x) = \tfrac{1}{(x-1)^2\,(x^2+1)^2}((x+1)^2\,(x^3+x^2+1)^2\,x^{8n+1} - x^{11} - 4x^8 - 3x^7 -$$
$$6x^6 - 10x^5 - 4x^4 - 9x^3 + 2x^2 - 3x - 2n\,(x-1)\,(x^2+1)$$
$$(2x^9 + 2x^8 + 2x^7 + 2x^6 + 8x^5 + 11x^4 + 9x^3 + 21x^2 + 3x + 12) + 2)$$

$$H(B_{6n+1}, x) =$$
$$\tfrac{1}{(x-1)^2\,(x^2+1)^2}((x+1)^2\,(x^2+x+1)\,(x^3+x^2+1)\,x^{8n+3} - x^{10} - x^9 - 7x^8 -$$
$$5x^7 - 7x^6 - 14x^5 + 3x^4 - 16x^3 + 12x^2 - 6x - 2n\,(x-1)\,(x^2+1)$$
$$(2x^9 + 2x^8 + 2x^7 + 2x^6 + 8x^5 + 11x^4 + 9x^3 + 21x^2 + 3x + 12) + 6)$$

$$H(B_{6n+2}, x) =$$
$$\tfrac{1}{(x-1)^2\,(x^2+1)^2}((x+1)^2\,(x^3+x+1)\,(x^3+x^2+1)\,x^{8n+4} - x^{12} - x^{11} -$$
$$2x^{10} - 8x^8 - 5x^7 - 8x^6 - 20x^5 + 9x^4 - 23x^3 + 22x^2 - 9x - 2n\,(x-1)$$
$$(x^2+1)\,(2x^9 + 2x^8 + 2x^7 + 2x^6 + 8x^5 + 11x^4 + 9x^3 + 21x^2 + 3x +$$
$$12) + 10)$$

$H(B_{6n+3},x) =$

$\frac{1}{(x-1)^2(x^2+1)^2}((x+1)^2(x^3+x^2+1)^2x^{8n+5} - 2x^{12} - x^{11} - 2x^{10} - 10x^8 -$
$6x^7 - 10x^6 - 25x^5 + 16x^4 - 30x^3 + 32x^2 - 12x - 2n(x-1)(x^2+1)$
$(2x^9 + 2x^8 + 2x^7 + 2x^6 + 8x^5 + 11x^4 + 9x^3 + 21x^2 + 3x + 12) + 14)$

$H(B_{6n+4},x) =$

$\frac{1}{(x-1)^2(x^2+1)^2}((x+1)^2(x^2+x+1)(x^3+x^2+1)x^{8n+7} - 2x^{12} - 3x^{10} -$
$x^9 - 13x^8 - 8x^7 - 11x^6 - 29x^5 + 23x^4 - 37x^3 + 42x^2 - 15x -$
$2n(x-1)(x^2+1)(2x^9 + 2x^8 + 2x^7 + 2x^6 + 8x^5 + 11x^4 + 9x^3 + 21x^2 +$
$3x + 12) + 18)$

$H(B_{6n+5},x) =$

$\frac{1}{(x-1)^2(x^2+1)^2}((x+1)^2(x^3+x+1)(x^3+x^2+1)x^{8n+8} - 3x^{12} - x^{11} -$
$4x^{10} - 14x^8 - 8x^7 - 12x^6 - 35x^5 + 29x^4 - 44x^3 + 52x^2 - 18x -$
$2n(x-1)(x^2+1)(2x^9 + 2x^8 + 2x^7 + 2x^6 + 8x^5 + 11x^4 + 9x^3 + 21x^2 +$
$3x + 12) + 22)$

$n \geq 1: \quad W(B_{6n}) = 768n^3 + 672n^2 + 28n - 7$

$W(B_{6n+1}) = 768n^3 + 1056n^2 + 284n + 27$

$W(B_{6n+2}) = 768n^3 + 1440n^2 + 732n + 109$

$W(B_{6n+3}) = 768n^3 + 1824n^2 + 1276n + 271$

$W(B_{6n+4}) = 768n^3 + 2208n^2 + 1916n + 529$

$W(B_{6n+5}) = 768n^3 + 2592n^2 + 2748n + 931$

References

[1] H. Hosoya, *Discrete Appl. Math.* **19** (1988) 239.

[2] M. Lepović and I. Gutman, *J. Chem. Inf. Comput. Sci.* **38** (1998) 823.

[3] G. Caporossi, A. A. Dobrynin, I. Gutman and P. Hansen, *Graph Theory Notes New York* **37** (1999) 10.

[4] I. Gutman, *Publ. Elektrotehn. Fak. (Beograd) Ser. Mat.* **10** (1999) 53.

[5] D. Stevanović, *Discrete Math.* in press.

[6] B. E. Sagan, Y. N. Yeh and P. Zhang, *Int. J. Quantum Chem.* **60** (1996) 959.

[7] I. Gutman, *Graph Theory Notes New York* **25** (1993) 13.

[8] A. A. Dobrynin, *Vychisl. Sistemy* **151** (1994) 37.

[9] A. A. Dobrynin, *Graph Theory Notes New York* **27** (1994) 50.

[10] I. Gutman, E. Estrada and O. Ivanciuc, *Graph Theory Notes New York* **36** (1999) 7.

[11] I. Gutman and S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer–Verlag, Berlin, 1989.

[12] E. Estrada, O. Ivanciuc, I. Gutman, A. Gutierrez, L. Rodriguez, New J. Chem. 22 (1998) 819.

[13] E. V. Konstantinova, M. V. Diudea, Croat. Chem. Acta 73 (2000) 383.

[14] I. Gutman and O. E. Polansky, *Commun. Math. Chem. (MATCH)* **20** (1986) 115.

[15] O. E. Polansky, M. Randić and H. Hosoya, *Commun. Math. Chem. (MATCH)* **24** (1989) 3.

[16] T. H. M. Smits, *Indag. Mathem., N.S.* **2** (1991) 359.