

Computing the Hosoya Polynomial of Graphs from Primary Subgraphs

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Abstract

The Hosoya polynomial of a graph encompasses many of its metric properties, for instance the Wiener index (alias average distance) and the hyper-Wiener index. An expression is obtained that reduces the computation of the Hosoya polynomial of a graph with cut vertices to the Hosoya polynomial of the so-called primary subgraphs. The main theorem is applied to specific constructions including bouquets of graphs, circuits of graphs, chains of graphs, and link of graphs. This is in turn applied to obtain the Hosoya polynomial of several chemically relevant families of graphs. In this way numerous known results are generalized and an approach to obtain them is simplified. Along the way several misprints from the literature are corrected.

1 Introduction

The Hosoya polynomial of a graph was introduced in Hosoya's seminal paper [23] back in 1988 and received a lot of attention afterwards. Actually, it was anticipated already in 1961 in a more general framework by Altenburg [2]; see the recent book chapter [22] on the historical developments and the relations between the Altenburg's multilinear form (also called *Altenburg polynomial*) and the Hosoya polynomial. The latter polynomial was later independently introduced and considered by Sagan, Yeh, and Zhang [31] under the

name *Wiener polynomial of a graph*. Both names are still used for the polynomial but the term Hosoya polynomial is nowadays used by the majority of researchers.

The main advantage of the Hosoya polynomial is that it contains a wealth of information about distance based graph invariants. For instance, knowing the Hosoya polynomial of a graph, it is straightforward to determine the famous Wiener index of a graph as the first derivative of the polynomial, evaluated at 1. Cash [7] noticed that the hyper-Wiener index can be obtained from the Hosoya polynomial in a similar simple manner, while Brückler et al. [5] reported the same for the Tratch-Stankevich-Zefirov index, cf. [22, Eq. (18)].

The Hosoya polynomial has been by now investigated on (in the historical order) trees [6, 19], composite graphs [32, 14, 15], benzenoid graphs [20, 36], tori [13], zig-zag open-ended nanotubes [38], certain graph decorations [39], armchair open-ended nanotubes [34], zigzag polyhex nanotorus [16], $TUC_4C_8(S)$ nanotubes [37], pentachains [1], polyphenyl chains [27], the circumcoronene series [28], as well as on Fibonacci and Lucas cubes [26] and Hanoi graphs [30]. For relations to other graph polynomials see [4, 21].

In this paper we consider the Hosoya polynomial on graphs that contain cut-vertices. Such graphs can be decomposed into subgraphs that we call *primary subgraphs*. Blocks of graphs are particular examples of primary subgraphs, but a primary subgraph may consist of several blocks. (For graph-theory concepts not defined here, such as cut-vertices and blocks, see any standard graph theory book, say [33].) In our main result, the Hosoya polynomial of a graph is expressed in terms of the Hosoya polynomial of the corresponding primary subgraphs. A related result for the Wiener index of a graph (in terms of the block-cut-vertex tree of the graph) was obtained in [3]. Our main result can be thus considered as an extension (and a simplification) of [3, Theorem 1]. In the case when a graph is decomposed into two primary subgraphs, our result is a special case of [35, Theorem 2.1] where a formula is given for the Hosoya polynomial of the gated amalgamation of two graphs, which is in turn a generalization of the corresponding result on the Wiener index [25]. On the other hand, [35, Corollary 2.1] is a special case of our main result.

We point out that our formulae require the knowledge of the Hosoya polynomials of the primary subgraphs, the so-called partial Hosoya polynomials, and specific distances. In many cases these are known or easy to find; especially in the case of bouquets, circuits, chains, and links when—to make things easier—the blocks are very often identical graphs. Very often authors go through several pages of computations to find only the Wiener index

of a family of graphs; one of the point of the present paper is to show that with much less effort one can find the Hosoya polynomial.

We proceed as follows. In the rest of this section the Hosoya polynomial and other concepts needed are formally introduced, while in the next section the main result is stated and proved. In Section 3 the result is applied to bouquets of graphs, circuits of graphs, chains of graphs, and links of graphs. These results are then applied in the final section to several families of graphs that appear in chemistry. Their Wiener index and hyper-Wiener index are obtained as a side product.

Let G be a connected graph and let $d(G, k)$, $k \geq 0$, be the number of vertex pairs at distance k . Then the *Hosoya polynomial* [23] of G is defined as

$$H(G, t) = \sum_{k \geq 1} d(G, k) t^k.$$

Before we continue, we point out that some authors define the Hosoya polynomial by adding in the above expression also the constant term $d(G, 0) = |V(G)|$. For our purposes the present definition is more convenient. Clearly, no matter which definition is selected, the considerations are equivalent.

We will write $d_G(u, v)$ for the usual shortest-path distance between u and v in G . If there will be only one graph in question, we will shorten the notation to $d(u, v)$. Let H_1 and H_2 be subgraphs of a connected graph G . Then the distance $d_G(H_1, H_2)$ between H_1 and H_2 is $\min\{d(u, v) \mid u \in V(H_1), v \in V(H_2)\}$. The *diameter* of G is defined as $\text{diam}(G) = \max_{u, v \in V(G)} d(u, v)$. For a finite set A and a nonnegative integer k let $\binom{A}{k}$ denote the set of all k -subsets of A . Note that $|\binom{A}{k}| = \binom{|A|}{k}$. With these notations at hand $H(G, t)$ can be more specifically written as

$$H(G, t) = \sum_{k=1}^{\text{diam}(G)} d(G, k) t^k = \sum_{\{u, v\} \in \binom{V(G)}{2}} t^{d(u, v)}.$$

Recall that the *Wiener index* $W(G)$ of G is defined by

$$W(G) = \sum_{\{u, v\} \in \binom{V(G)}{2}} d(u, v),$$

and that the *hyper-Wiener index* $WW(G)$ is

$$WW(G) = \frac{1}{2} \sum_{\{u, v\} \in \binom{V(G)}{2}} (d(u, v) + d(u, v)^2).$$

The relations between the Hosoya polynomial and these two indices are then

$$W(G) = \left. \frac{dH(G, t)}{dt} \right|_{t=1} \quad \text{and} \quad WW(G) = \left. \frac{dH(G, t)}{dt} \right|_{t=1} + \frac{1}{2} \cdot \left. \frac{d^2 H(G, t)}{dt^2} \right|_{t=1}.$$

Finally, for a positive integer n we will use the notation $[n] = \{1, 2, \dots, n\}$.

2 Main result

Let G be a connected graph and let $u \in V(G)$. Then the *partial Hosoya polynomial with respect to u* is

$$H_u(G, t) = \sum_{\substack{v \in V(G) \\ v \neq u}} t^{d(u, v)}.$$

This concept was used by Došlić in [14] under the name *partial Wiener polynomial*.

Let G be a connected graph constructed from pairwise disjoint connected graphs G_1, \dots, G_k as follows. Select a vertex of G_1 , a vertex of G_2 , and identify these two vertices. Then continue in this manner inductively. More precisely, suppose that we have already used G_1, \dots, G_i in the construction, where $2 \leq i \leq k - 1$. Then select a vertex in the already constructed graph (which may in particular be one of the already selected vertices) and a vertex of G_{i+1} ; we identify these two vertices. Note that the graph G constructed in this way has a tree-like structure, the G_i 's being its building stones (see Fig. 1). We will briefly say that G is obtained by *point-attaching* from G_1, \dots, G_k and that G_i 's are the *primary subgraphs* of G . A particular case of this construction is the decomposition of a connected graph into blocks.

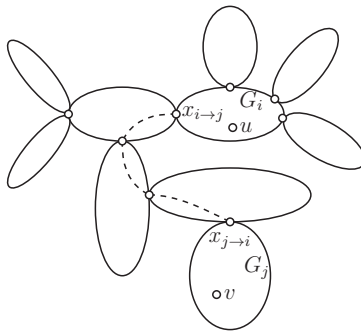


Figure 1: Graph G obtained by point-attaching from G_1, \dots, G_k

Let G be a graph obtained by point-attaching from G_1, \dots, G_k . Then let $\delta_{ij} = d_G(G_i, G_j)$. This distance is realized by precisely one vertex from G_i and one vertex

from G_j , denote them with $x_{i \rightarrow j}$ and $x_{j \rightarrow i}$, respectively; see Fig. 1 where the distance between G_i and G_j is indicated with a dashed line. Note that if G_i and G_j share a vertex x , then $x = x_{i \rightarrow j} = x_{j \rightarrow i}$ and $\delta_{ij} = 0$.

Now everything is ready for our main result.

Theorem 2.1 *Let G be a connected graph obtained by point-attaching from G_1, \dots, G_k , and let $x_{i \rightarrow j}$ and δ_{ij} be as above. Then*

$$H(G, t) = \sum_{i=1}^k H(G_i, t) + \sum_{\{i,j\} \in \binom{[k]}{2}} (H_{x_{i \rightarrow j}}(G_i, t) \cdot H_{x_{j \rightarrow i}}(G_j, t) \cdot t^{\delta_{ij}}). \quad (1)$$

Proof. Let $u \neq v$ be arbitrary vertices of G . We need to show that their contribution to the claimed expression is $t^{d(u,v)}$.

Suppose first that u and v belong to the same primary subgraph, say $u, v \in G_i$. Then $d_G(u, v) = d_{G_i}(u, v)$ and hence $t^{d(u,v)}$ is included in the corresponding term of the first sum of the theorem.

Assume next that u and v do not belong to the same primary subgraph. If u or v is an attaching vertex, then it belongs to more than one primary subgraph. Hence select primary subgraphs G_i and G_j with $u \in G_i$ and $v \in G_j$ such that $\delta_{ij} = d_G(G_i, G_j)$. By our assumption $i \neq j$ and hence

$$d_G(u, v) = d_{G_i}(u, x_{i \rightarrow j}) + \delta_{ij} + d_{G_j}(x_{j \rightarrow i}, v),$$

cf. Fig. 1 again. It is possible that $\delta_{ij} = 0$, that is, $x_{i \rightarrow j} = x_{j \rightarrow i}$, but in any case $t^{d(u,v)}$ is a term in the product $H_{x_{i \rightarrow j}}(G_i, t) \cdot t^{\delta_{ij}} \cdot H_{x_{j \rightarrow i}}(G_j, t)$.

We have thus proved that for any distinct vertices u and v , the term $t^{d(u,v)}$ is included in the claimed expression. To complete the argument we need to show that no such term is included more than once. To verify this it suffices to prove that the total number of pairs of vertices considered in (1) is equal to the total number of pairs of vertices. Set $n_i = |V(G_i)| - 1$, $1 \leq i \leq k$, and note that then $|V(G)| = 1 + \sum_{i=1}^k n_i$. Then the first term of (1) involves

$$A = \sum_{i=1}^k \binom{n_i + 1}{2}$$

pairs of vertices, while the second sum involves

$$B = \sum_{\{i,j\} \in \binom{[k]}{2}} n_i n_j$$

pairs of vertices of G . Then

$$\begin{aligned} 2(A + B) &= \sum_{i=1}^k n_i^2 + \sum_{i=1}^k n_i + \sum_{\{i,j\} \in \binom{[k]}{2}} 2n_i n_j \\ &= \left(\sum_{i=1}^k n_i \right) \cdot \left(1 + \sum_{i=1}^k n_i \right) \\ &= (|V(G)| - 1) \cdot |V(G)|. \end{aligned}$$

We conclude that $A + B = \binom{|V(G)|}{2}$, that is, the number of pairs of vertices involved in (1) is equal to the number of all pairs. \square

As an example consider the graph $Q(m, n)$ constructed in the following manner: denoting by K_q the complete graph with q vertices, consider the graph K_m and m copies of K_n . By definition, the graph $Q(m, n)$ is obtained by identifying each vertex of K_m with a vertex of a unique K_n . The graph $Q(6, 4)$ is shown in Fig. 2.

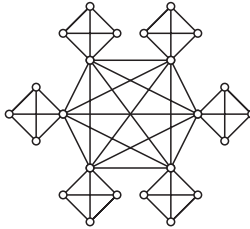


Figure 2: $Q(6, 4)$

Clearly, the Hosoya polynomial of K_q is $\frac{1}{2}q(q-1)t$ and the partial Hosoya polynomial with respect to any of its vertices is $(q-1)t$. The distance between the central K_m and a K_n is 0, while the distance between any two distinct K_n 's is 1. Now, Theorem 2.1 gives, after elementary calculations,

$$\begin{aligned} H(Q(m, n), t) &= \frac{1}{2}m(m+n^2-n-1)t \\ &\quad + m(m-1)(n-1)t^2 + \frac{1}{2}m(m-1)(n-1)^2t^3. \end{aligned}$$

For the Wiener index and the hyper-Wiener index we obtain

$$\begin{aligned} W(Q(m, n)) &= \frac{1}{2}mn(3mn - 2m - 2n + 1), \\ HW(Q(m, n)) &= \frac{1}{2}m(6mn^2 - 6mn - 5n^2 + m + 5n - 1). \end{aligned}$$

Notice that the Wiener index $W(Q(m, n))$ is symmetric in m and n .

3 Specific constructions

In this section we present several constructions of graphs to which our main result can be applied. These constructions will in turn be used in the next section where chemical applications will be given.

3.1 Bouquet of graphs

Let G_1, G_2, \dots, G_k be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. By definition, the bouquet G of the graphs $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i\}_{i=1}^k$ is obtained by identifying the vertices x_1, x_2, \dots, x_k (see Fig. 3 for $k = 3$).

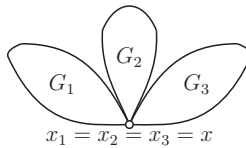


Figure 3: A bouquet of three graphs

Clearly, we have a graph obtained by point-attaching from G_1, G_2, \dots, G_k and formula (1) holds with $\tilde{\delta}_{ij} = 0$ and $x_{i \rightarrow j} = x_{j \rightarrow i} = x$, where x is the vertex obtained from the identification of the x_i 's. Formula (1) becomes

$$H(G, t) = \sum_{i=1}^k H(G_i, t) + \sum_{\{i,j\} \in \binom{[k]}{2}} H_x(G_i, t) \cdot H_x(G_j, t). \tag{2}$$

Consider the following special case of identical G_i 's. Let X be a connected graph and let $x \in V(X)$. Take $G_i = X$ and $x_i = x$ for $i \in [k]$. Formula (2) becomes

$$H(G, t) = kH(X, t) + \frac{1}{2}k(k-1)H_x^2(X, t). \tag{3}$$

3.2 Circuit of graphs

Let G_1, G_2, \dots, G_k be a finite sequence of pairwise disjoint connected graphs and let $x_i \in V(G_i)$. By definition, the circuit G of the graphs $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i\}_{i=1}^k$ is obtained by identifying the vertex x_i of the graph G_i with the i -th vertex of the cycle graph C_k (see Fig. 4 for $k = 4$).

The Hosoya polynomial of G is given by

$$H(G, t) = \sum_{i=1}^k H(G_i, t) + \sum_{\{i,j\} \in \binom{[k]}{2}} t^{\min(j-i, k-j+i)} (1 + H_{x_i}(G_i, t)) (1 + H_{x_j}(G_j, t)). \tag{4}$$

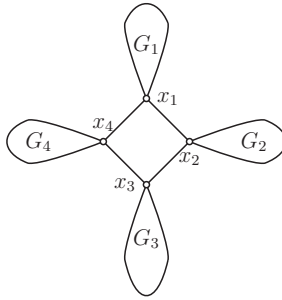


Figure 4: A circuit of four graphs

This can be derived from Theorem 2.1 by viewing G as a graph obtained by point-attaching from the $k + 1$ graphs G_1, G_2, \dots, G_k , and C_k . However, we prefer to give a direct proof.

Let $u \neq v$ be arbitrary vertices in G . Suppose first that u and v belong to the same graph G_i . In this case, $t^{d(u,v)}$ is included in the corresponding term of the first sum in (4). Assume now that $u \in G_i$ and $v \in G_j$, $i < j$. Then $d(u, v) = d(u, x_i) + d(x_i, x_j) + d(x_j, v)$, where $d(x_i, x_j) = \min(j - i, k - j + i)$. The first and the last term of this sum may be equal to 0. It follows that $t^{d(u,v)}$ is a term in the product under the 2nd sum in (4). To complete the argument we need to show that no such term is included more than once. To verify this it suffices to prove that the total number of pairs of vertices considered in (4) is equal to the total number of pairs of vertices. Setting $n_i = |V(G_i)|$, the number of pairs of vertices involved in the right-hand side of (4) is $\frac{1}{2} \sum_{i=1}^k n_i(n_i - 1) + \sum_{\{i,j\} \in \binom{[k]}{2}} n_i n_j = \frac{1}{2} \left(\sum_{i=1}^k n_i \right) \left(\sum_{i=1}^k n_i - 1 \right)$, i.e. the number of all unordered pairs of distinct vertices in G .

Consider the following special case of identical G_i 's. Let X be a connected graph and let $x \in V(X)$. Take $G_i = X$, $x_i = x$ for $i \in [k]$. Then formula (4) becomes

$$H(G, t) = kH(X, t) + (1 + H_x(X, t))^2 H(C_k, t). \tag{5}$$

3.3 Chain of graphs

Let G_1, G_2, \dots, G_k be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. By definition (see [29]) the chain G of the graphs $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i, y_i\}_{i=1}^k$ is obtained by identifying the vertex y_i with the vertex x_{i+1} for $i \in [k - 1]$ (see Fig. 5 for $k = 4$).

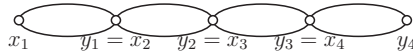


Figure 5: A chain of four graphs

Denoting $d_l = d(x_l, y_l)$, we define

$$s_{i,j} = \begin{cases} d_{i+1} + d_{i+2} + \dots + d_{j-1} & \text{if } j - i \geq 2, \\ 0 & \text{otherwise.} \end{cases} \quad (6)$$

Clearly, we have a graph obtained by point-attaching from G_1, \dots, G_k and formula (1) holds with $x_{i \rightarrow j} = y_i, x_{j \rightarrow i} = x_j$, and $\delta_{ij} = s_{ij}$. Consequently, we have

$$H(G, t) = \sum_{i=1}^k H(G_i, t) + \sum_{\{i,j\} \in \binom{[k]}{2}} H_{y_i}(G_i, t) H_{x_j}(G_j, t) t^{s_{i,j}}. \quad (7)$$

Consider the following special case of identical G_i 's. Let X be a connected graph and let $x, y \in V(X)$. Take $G_i = X, x_i = x, y_i = y$ for $i \in [k]$. Then, denoting $d = d(x, y)$, we have $s_{i,j} = (j - i - 1)d$ and formula (7) becomes

$$H(G, t) = kH(X, t) + H_x(X, t)H_y(X, t) \frac{t^{kd} - kt^d + k - 1}{(t^d - 1)^2}. \quad (8)$$

We mention that in [29] long expressions with long proofs are given for the Wiener index (pp. 86–89) and for the hyper-Wiener index (pp. 93–94) of a chain of graphs.

3.4 Link of graphs

Let G_1, G_2, \dots, G_k be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. The link G of the graphs $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i, y_i\}_{i=1}^k$ is obtained by joining by an edge the vertex y_i of G_i with the vertex x_{i+1} of G_{i+1} for all $i = 1, 2, \dots, k - 1$ (see Fig. 6 for $k = 4$).

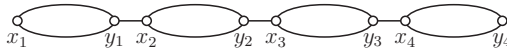


Figure 6: A link of four graphs

The Hosoya polynomial of G is given by

$$H(G, t) = \sum_{i=1}^k H(G_i, t) + \sum_{\{i,j\} \in \binom{[k]}{2}} (1 + H_{y_i}(G_i, t)) (1 + H_{x_j}(G_j, t)) t^{j-i+s_{i,j}}, \quad (9)$$

where s_{ij} is defined in (6), with $d_l = d(x_l, y_l)$.

Formula (9) can be derived from Theorem 2.1 by viewing G as a chain of $2k - 1$ graphs: the k G_i 's alternating with the $k - 1$ K_2 's (edges). This derivation is rather cumbersome and, consequently, we prefer to give a direct proof.

Let $u \neq v$ be arbitrary vertices in G . Suppose first that u and v belong to the same graph G_i . In this case, $t^{d(u,v)}$ is included in the corresponding term of the first sum in (9). Assume now that $u \in G_i$ and $v \in G_j$, $i < j$. We break up $d(u, v)$ into three parts: $d(u, y_i)$, $d(y_i, x_j) = j - i + s_{i,j}$, and $d(x_j, v)$. The first and the last part may be equal to 0. It follows that $t^d(u, v)$ is a term in the product under the 2nd sum in (9). Using the same reasoning as for the circuit of graphs we then infer that the number of pairs of vertices involved in the right-hand side in (9) is equal to the number of all unordered pairs of distinct vertices in G .

Consider the following special case of identical G_i 's. Let X be a connected graph and let $x, y \in V(X)$. Take $G_i = X$, $x_i = x$, $y_i = y$ for all $i \in [k]$. Then, denoting $d = d(x, y)$, we have $d_1 = d_2 = \dots = d_k = d$ and formula (9) becomes

$$H(G, t) = kH(X, t) + (1 + H_x(X, t))(1 + H_y(X, t)) \frac{t^{kd+k+1} - kt^{d+2} + kt - t}{(t^{d+1} - 1)^2}. \quad (10)$$

4 Chemical applications

In this section we apply our previous results in order to obtain the Hosoya polynomial of families of graphs that are of importance in chemistry. As already pointed out, numerous distance-based invariants such as the Wiener and the hyper-Wiener index can then be routinely derived.

4.1 Spiro-chains

Spiro-chains are defined in [12, p.114]. Making use of the concept of chain of graphs, a spiro-chain can be defined as a chain of cycles. We denote by $S_{q,h,k}$ the chain of k cycles C_q in which the distance between two consecutive contact vertices is h (see $S_{6,2,5}$ in Fig. 7).

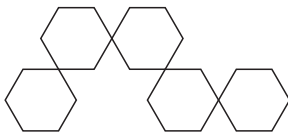


Figure 7: Spiro-chain $S_{6,2,5}$

The Hosoya polynomial of $S_{q,h,k}$ can be easily obtained from (8). We distinguish two cases: q odd and q even.

Assume q is odd: $q = 2r + 1$ ($r \geq 1$). In (8) we take $g = C_q$ and $d = h$. We have $H(C_q, t) = (2r + 1) \sum_{j=1}^r t^j$ [31] and $H_x(C_q, t) = 2 \sum_{j=1}^r t^j$ for any vertex x of C_q . Now, (8) yields

$$H(S_{2r+1,h,k}, t) = \frac{k(2r+1)t(t^r-1)}{t-1} + \frac{4t^2(t^r-1)^2(t^{kh}-kt^h+k-1)}{(t-1)^2(t^h-1)^2}.$$

For the Wiener index and the hyper-Wiener index we obtain

$$W(S_{2r+1,h,k}) = \frac{1}{6}kr[3(r+1)(1-2r+4kr) + 4rh(k-1)(k-2)], \quad (11)$$

$$WW(S_{2r+1,h,k}) = \frac{1}{6}kr[(r+1)(2-6r+11kr+7kr^2-5r^2) + 2rh(k-1)(k-2)(2r+3) + rh^2(k-1)^2(k-2)]. \quad (12)$$

Assume q is even: $q = 2r$ ($r \geq 1$). Again in (8) we take $g = C_q$ and $d = h$. We have $H(C_q, t) = 2r \sum_{j=1}^{r-1} t^j + rt^r$ [31] and $H_x(C_q, t) = 2 \sum_{j=1}^{r-1} t^j + t^r$ for any vertex x of C_q . Now, (8) yields

$$H(S_{2r,h,k}, t) = \frac{kr(t^{r+1}+t^r-2t)}{t-1} + \frac{(t^{r+1}+t^r-2t)^2(t^{kh}-kt^h+k-1)}{(t-1)^2(t^h-1)^2}.$$

For the Wiener index and the hyper-Wiener index we obtain

$$W(S_{2r+1,h,k}) = \frac{1}{6}k[h(2r-1)^2(k-1)(k-2) + 6r^2(1-r+2rk-k)], \quad (13)$$

$$WW(S_{2r+1,h,k}) = \frac{1}{6}kr[(r+1)(2-6r+11kr+7kr^2-5r^2) + 2rh(k-1)(k-1)(2r+3) + rh^2(k-1)^2(k-2)]. \quad (14)$$

From Eqs. (11), (12), (13), (14), setting $q = 3, 4, 5, 6$ and $h \in \{1, 2, \dots, \lfloor \frac{q}{2} \rfloor\}$, we recover all the expressions in Table 4.2 of [12, p.115] (they occur also in [11]). Incidentally, there is a typo in the last expression of Table 4.2 of [12]: 847 should be changed to 874. The corresponding expression in [11, Eq. (64)] is correct.

4.2 Polyphenylenes

Similarly to the above definition of the spiro-chain $S_{q,h,k}$, we can define the graph $L_{q,h,k}$ as the link of k cycles C_q in which the distance between the two contact vertices in the same cycle is h . See Fig. 8 for $L_{6,2,5}$.

We consider here only the case of hexagons ($q = 6$), the so-called ortho-, meta-, or para-polyphenyl chains, corresponding to $h = 1, 2$ or 3 , respectively (see [9, 10]).

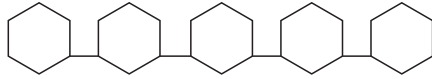


Figure 8: $L_{6,2,5}$

If in (10) we take $H(X, t) = 6t + 6t^2 + 3t^3$ (the Hosoya polynomial of C_6) and $H_x(X, t) = H_y(X, t) = 2t + 2t^2 + t^3$ (the relative Hosoya polynomial of C_6 with respect to any of its vertices), then (10) becomes

$$H(L_{6,h,k}, t) = 3kt(2 + 2t + t^2) + \frac{(t + 1)^2(t^2 + t + 1)^2(t^{h+k+1} - kt^{h+2} + kt - t)}{(t^{h+1} - 1)^2}.$$

The expression obtained from here for all the possible values $h = 1, 2, 3$ have been obtained by a different method in [27] (Theorems 2.1, 2.2, and 2.3).

Now, for the Wiener index and the hyper-Wiener index we obtain

$$\begin{aligned} W(L_{6,h,k}) &= 3k[4h - 11 + 6k(3 - h) + 2k^2(1 + h)], \\ WW(L_{6,h,k}) &= \frac{3}{2}k[-2h^2 + 32h - 69 + k(5h^2 - 44h + 82) \\ &\quad - 2k^2(h + 1)(2h - 7) + k^3(h + 1)^2]. \end{aligned} \tag{15}$$

Setting $h = 1, 2, 3$ in (15), we recover the expressions given in [10, Corollary 3.3]. The Wiener index of $L_{6,3,k}$ is found also in [9, p.1233]. However, the formulation of the final result has a typo: the binomial $\binom{n+1}{3}$ should be preceded by 144.

The reader may be interested to find in the same way the Hosoya polynomial, the Wiener index, and the hyper-Wiener index of $L_{q,h,k}$.

4.3 Nanostar dendrimers

We intend to derive the Hosoya polynomial of the nanostar dendrimer D_k defined pictorially in [17]. A better pictorial definition can be found in [18]. In order to define D_k , first we define recursively an auxiliary family of rooted dendrimers G_k ($k \geq 1$). We need a fixed graph F defined in Fig. 9; we consider one of its endpoint to be the root of F . The graph G_1 is defined in Fig. 10, the leaf being its root. Now we define G_k ($k \geq 2$) as the bouquet of the following 3 graphs: G_{k-1}, G_{k-1} , and F with respect to their roots; the root of G_k is taken to be its unique leaf (see G_2 and G_3 in Fig. 11). Finally, we define D_k ($k \geq 1$) as the bouquet of 3 copies of G_k with respect to their roots (D_2 is shown in Fig. 12, where the circles represent hexagons).

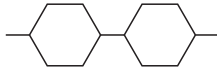


Figure 9: Graph F

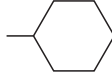


Figure 10: Graph G_1

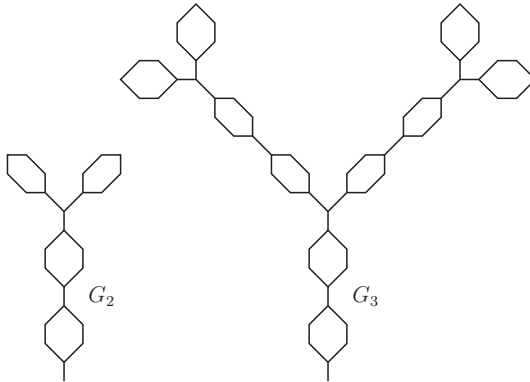


Figure 11: Graphs G_2 and G_3

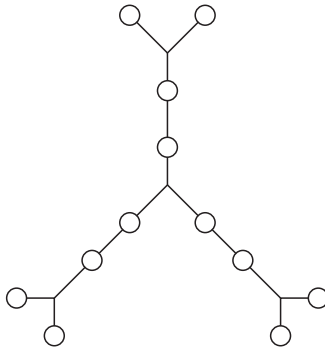


Figure 12: Nanostar D_2

Let s denote the partial Hosoya polynomial of the graph F with respect to its root and let p denote the Hosoya polynomial of F . Direct computation yields

$$\begin{aligned}
 s &= t^9 + t(1+t)(1+t+t^2)(1+t^4), \\
 p &= 15t + 20t^2 + 18t^3 + 12t^4 + 10t^5 + 8t^6 + 5t^7 + 2t^8 + t^9.
 \end{aligned}
 \tag{16}$$

Let r_k denote the partial Hosoya polynomial of G_k with respect to its root. It is straightforward to find $r_1 = t(1+t)(1+t+t^2)$ and the recurrence relation $r_k = s + 2t^9 r_{k-1}$; they lead to

$$r_k = s \frac{(2t^9)^{k-1} - 1}{2t^9 - 1} + (2t^9)^{k-1} t(1+t)(1+t+t^2). \quad (17)$$

Now from (2) we obtain a recurrence relation for $H(G_k, t)$:

$$H(G_k, t) = 2H(G_{k-1}, t) + p + 2sr_{k-1} + r_{k-1}^2,$$

the initial condition being

$$H(G_1, t) = 7t + 8t^2 + 5t^3 + t^4. \quad (18)$$

The solution is

$$H(G_k, t) = 2^{k-1}(p + H(G_1, t)) - p + \sum_{j=1}^{k-1} 2^{k-1-j} r_j (2s + r_j), \quad (19)$$

where p and $H(G_1, t)$ are given in (16) and (18), respectively.

Although not required in the sequel, we give the Wiener index and the hyper-Wiener index of G_k :

$$\begin{aligned} W(G_k) &= 1323 + 2^{k-1}3735 - 2^{2k-2}12711 + 2^k 2223k + 2^{2k-2}3249k, \\ WW(G_k) &= -45867 - 2^{k-1}173401 + 2^{2k-3}1060083 - 2^{k-1}132777k \\ &\quad - 2^{2k-3}454347k + 20007k^2 2^{k-1} + 29241k^2 2^{2k-2}. \end{aligned}$$

Since D_k is a bouquet of three copies of G_k with respect to their roots, from (3) we have

$$H(D_k, t) = 3H(G_k, t) + 3r_k^2,$$

where the terms in the right-hand side are given in (19) and (17). For the Wiener index and the hyper-Wiener index of D_k we obtain

$$\begin{aligned} W(D_k) &= -9369 - 2^{2k-2}75411 + 2^{2k-2}29241k + 2^{k-1}56205, \\ WW(D_k) &= 116340 - 2^{k-1}1429983 + 2^{2k-3}4790367 - 2^{2k-3}2685555k \\ &\quad + 2^{2k-2}263169k^2. \end{aligned}$$

Incidentally, the formula given in [17, p.62] for the Wiener index of D_n contains some misprints; for example, for D_1 it does not give the correct value 666 found on p. 60.

4.4 Triangulanes

We intend to derive the Hosoya polynomial of the triangulane T_k defined pictorially in [24]. We define T_k recursively in a manner that will be useful in our approach. First we define recursively an auxiliary family of triangulanes G_k ($k \geq 1$). Let G_1 be a triangle and denote one of its vertices by y_1 . We define G_k ($k \geq 2$) as the circuit of the graphs G_{k-1}, G_{k-1} , and K_1 and denote by y_k the vertex where K_1 has been placed. The graphs G_1, G_2, G_3 are shown in Fig. 13.

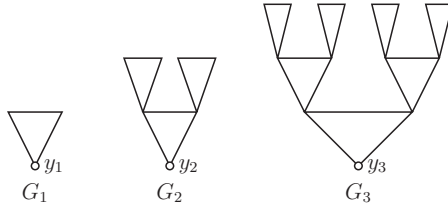


Figure 13: Graphs G_1, G_2, G_3

Now, T_k is defined as the circuit of 3 copies of G_k with respect to their vertices y_k (T_2 is shown in Fig. 14).

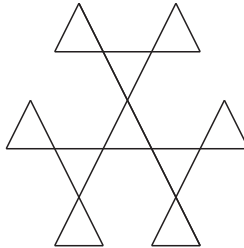


Figure 14: Graph T_2

Let r_k denote the partial Hosoya polynomial of G_k with respect to the vertex y_k . It is straightforward to derive that

$$1 + r_k = \frac{2^{k+1}t^{k+1} - 1}{2t - 1}. \tag{20}$$

Since G_k is the circuit of the graphs G_{k-1}, G_{k-1} , and K_1 , from (4) we obtain the recurrence equation

$$H(G_k, t) = 2H(G_{k-1}, t) + t(1 + r_{k-1})^2 + 2t(1 + r_{k-1}).$$

The initial condition is $H(G_1, t) = 3t$ and the solution is found to be

$$H(G_k, t) = \frac{2^{k+2}t^{k+2} + 4t^2 - 3t}{(2t - 1)^2} - \frac{2^k(4t^2 + 3t)}{2t^2 - 1} + \frac{2^{2k+1}t^{2k+3}}{(2t - 1)^2(2t^2 - 1)}. \quad (21)$$

Although not required in the sequel, we give the Wiener index and the hyper-Wiener index of G_k :

$$\begin{aligned} W(G_k) &= 2^{2k+1}(2k - 5) + 2^k(4k + 9) + 1, \\ WW(G_k) &= 2^{2k+1}(2k^2 - 9k + 16) + 2^k(2k^2 - 6k - 29) - 3. \end{aligned}$$

Since T_k is a circuit of 3 copies of G_k with respect to the vertices y_k , from (5) we obtain

$$H(T_k, t) = 3H(G_k, t) + 3t(1 + r_k)^2,$$

where the expressions occurring in the right-hand side are given in (21) and (20). We obtain easily

$$H(T_k, t) = \frac{6t}{2t - 1} - \frac{2^n 3t(4t + 3)}{2t^2 - 1} + \frac{2^{2n+1} 3t^{2n+3}(2t + 1)}{(2t - 1)(2t^2 - 1)}.$$

For the Wiener index of T_k we obtain

$$W(T_k) = 2^{2n+1}3(6n - 7) + 2^n 51 - 6.$$

This expression can be found in [24, Theorem 1] and in [8, p.37, Theorem 5]. For the hyper-Wiener index of T_k we have

$$WW(T_k) = 2^{2n+1}3(6n^2 - 11n + 20) - 2^n 123 + 6.$$

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References

- [1] A. A. Ali, A. M. Ali, Hosoya polynomials of pentachains, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 807–819.
- [2] K. Altenburg, Zur Berechnung des Radius verzweigter Moleküle, *Kolloid Z.* **178** (1961) 112–119.
- [3] R. Balakrishnan, N. Sridharan, K. Viswanathan Iyer, Wiener index of graphs with more than one cut-vertex, *Appl. Math. Lett.* **21** (2008) 922–927.
- [4] A. Behmaram, H. Yousefi-Azari, A. R. Ashrafi, Some new results on distance-based polynomials, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 39–50.

- [5] F. M. Brückler, T. Došlić, A. Graovac, I. Gutman, On a class of distance-based molecular structure descriptors, *Chem. Phys. Lett.* **503** (2011) 336–338.
- [6] G. Caporossi, A. A. Dobrynin, I. Gutman, P. Hansen, Trees with palindromic Hosoya polynomials, *Graph Theory Notes New York* **37** (1999) 10–16.
- [7] G. G. Cash, Relationship between the Hosoya polynomial and the hyper-Wiener index, *Appl. Math. Lett.* **15** (2002) 893–895.
- [8] F. Cataldo, A. Graovac, O. Ori (Eds.), *The Mathematics and Topology of Fullerenes*, Springer, Dordrecht, 2011.
- [9] M. R. Darafsheh, Computation of topological indices of some graphs, *Acta Appl. Math.* **110** (2010) 1225–1235.
- [10] H. Deng, Wiener indices of spiro and polyphenyl hexagonal chains, *Math. Comput. Model.* **55** (2012) 634–644.
- [11] M. V. Diudea, G. Katona, O. M. Minailiuc, B. Parv, Wiener and hyper-Wiener indices in spiro-graphs, *Russian Chem. Bull.* **44** (1995) 1606–1611.
- [12] M. V. Diudea, I. Gutman, J. Lorentz, *Molecular Topology*, Nova, Huntington, 2001.
- [13] M. V. Diudea, Hosoya polynomial in tori, *MATCH Commun. Math. Comput. Chem.* **45** (2002) 109–122.
- [14] T. Došlić, Vertex-weighted Wiener polynomials for composite graphs, *Ars Math. Contemp.* **1** (2008) 66–80.
- [15] M. Eliasi, A. Iranmanesh, Hosoya polynomial of hierarchical product of graphs, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 111–119.
- [16] M. Eliasi, B. Taeri, Hosoya polynomial of zigzag polyhex nanotorus, *J. Serb. Chem. Soc.* **73** (2008) 311–319.
- [17] M. Ghorbani, M. Songhori, Some topological indices of nanostar dendrimers, *Iranian J. Math. Chem.* **1** (2010) 57–65.
- [18] M. Ghorbani, A. Mohammadi, F. Madadi, Some topological indices of nanostar dendrimers, *Optoelectr. Adv. Mater. Rapid Comm.* **4** (2010) 1871–1873.
- [19] I. Gutman, Some relations between distance-based polynomials of trees, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)* **131** (2005) 1–7.
- [20] I. Gutman, S. Klavžar, M. Petkovšek, P. Žigert, On Hosoya polynomials of benzenoid graphs, *MATCH Commun. Math. Comput. Chem.* **43** (2001) 49–66.
- [21] I. Gutman, O. Miljković, B. Zhou, M. Petrović, Inequalities between distance-based graph polynomials, *Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.)* **133** (2006) 57–68.

- [22] I. Gutman, Y. Zhang, M. Dehmer, A. Ilić, Altenburg, Wiener, and Hosoya polynomials, in: I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs — Theory*, Univ. Kragujevac, Kragujevac, 2012, pp. 49–70.
- [23] H. Hosoya, On some counting polynomials in chemistry, *Discr. Appl. Math.* **19** (1988) 239–257.
- [24] M. H. Khalifeh, H. Yousefi–Azari, A. R. Ashrafi, Computing Wiener and Kirchhoff indices of a triangulane, *Indian J. Chem.* **47A** (2008) 1503–1507.
- [25] S. Klavžar, Wiener index under gated amalgamations, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 181–194.
- [26] S. Klavžar, M. Mollard, Wiener index and Hosoya polynomial of Fibonacci and Lucas cubes, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 311–324.
- [27] X. Li, G. Wang, H. Bian, R. Hu, The Hosoya polynomial decomposition for polyphenyl chains, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 357–368.
- [28] X. Lin, S. J. Xu, Y. N. Yeh, Hosoya polynomials of circumcoronene series, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 755–763.
- [29] T. Mansour, M. Schork, Wiener, hyper–Wiener, detour and hyper–detour indices of bridge and chain graphs, *J. Math. Chem.* **47** (2010) 72–98.
- [30] P. K. Narayankar, S. B. Lokesh, V. Mathad, I. Gutman, Hosoya polynomial of Hanoi graphs, *Kragujevac J. Math.* **36** (2012) 51–57.
- [31] B. E. Sagan, Y. N. Yeh, P. Zhang, The Wiener polynomial of a graph, *Int. J. Quantum Chem.* **60** (1996) 959–969.
- [32] D. Stevanović, Hosoya polynomial of composite graphs, *Discr. Math.* **235** (2001) 237–244.
- [33] D. B. West, *Introduction to Graph Theory*, Prentice Hall, Upper Saddle River, 2001.
- [34] S. Xu, H. Zhang, Hosoya polynomials of armchair open–ended nanotubes, *Int. J. Quantum Chem.* **107** (2007) 586–596.
- [35] S. Xu, H. Zhang, Hosoya polynomials under gated amalgamations, *Discr. Appl. Math.* **156** (2008) 2407–2419.
- [36] S. Xu, H. Zhang, The Hosoya polynomial decomposition for catacondensed benzenoid graphs, *Discr. Appl. Math.* **156** (2008) 2930–2938.
- [37] S. Xu, H. Zhang, Hosoya polynomials of $TUC_4C_8(S)$ nanotubes, *J. Math. Chem.* **45** (2009) 488–502.
- [38] S. Xu, H. Zhang, M. V. Diudea, Hosoya polynomials of zig–zag open–ended nanotubes, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 443–456.
- [39] W. Yan, B.-Y. Yang, Y. N. Yeh, The behavior of Wiener indices and polynomials of graphs under five graph decorations, *Appl. Math. Lett.* **20** (2007) 290–295.