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A Method for Computing the Edge–Hosoya Polynomial with Application to Phenylenes

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Abstract

The edge-Hosoya polynomial of a graph is the edge version of the famous Hosoya polynomial. Therefore, the edge-Hosoya polynomial counts the number of (unordered) pairs of edges at distance $k \geq 0$ in a given graph. It is well known that this polynomial is closely related to the edge-Wiener index and the edge-hyper-Wiener index. As the main result of this paper, we greatly generalize an earlier result by providing a method for calculating the edge-Hosoya polynomial of a graph G which is obtained by identifying two edges of connected bipartite graphs G_1 and G_2. To show how the main theorem can be used, we apply it to phenylene chains. In particular, we present the recurrence relations and a linear time algorithm for calculating the edge-Hosoya polynomial of any phenylene chain. As a consequence, closed formula for the edge-Hosoya polynomial of linear phenylene chains is derived.

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1 Introduction

The Hosoya polynomial was introduced by H. Hosoya in 1988 under the name Wiener polynomial [11]. It is defined in such a way that the coefficient before x^k, $k \geq 0$, represents the number of (unordered) pairs of vertices at distance k in a given graph. This polynomial is of great importance in mathematical chemistry due to the fact that it is closely related to the famous Wiener index [16]. More precisely, the Wiener index of a graph can be easily calculated by using the derivative of the Hosoya polynomial. In addition, the hyper-Wiener index can also be easily obtained from the Hosoya polynomial [6].

Therefore, it is not surprising that in the past the Hosoya polynomial was considered in numerous papers. For example, the Hosoya polynomial was investigated for benzenoid (hexagonal) chains [10, 23–25], other important molecular graphs [17, 18, 26], Fibonacci and Lucas cubes [15]. Moreover, in [9, 24] the authors considered general situations in which the Hosoya polynomial can be computed by using subgraphs and in [19] the Hosoya polynomial of weighted graphs was investigated.

Later appeared also the edge versions of the above mentioned concepts, see [8, 12, 14] for the edge-Wiener index, [13] for the edge-hyper-Wiener index, and [4] for the edge-Hosoya polynomial. Especially the edge-Wiener index attracted quite a lot of attention, see [7, 20, 27] for an example of relevant recent investigations. Regarding the edge-Hosoya polynomial, the relation between this polynomial and the standard Hosoya polynomial for trees was deduced in [21]. Moreover, the edge-Hosoya polynomial of benzenoid chains was investigated in [22].

The aim of this paper is to develop a new method for computing the edge-Hosoya polynomial of any connected graph obtained from smaller graphs by identifying two edges, which greatly generalizes results from [22]. For the standard Hosoya polynomial, a more general result was proved in [24] by considering gated amalgams, but several additional insights are needed when dealing with distances between edges of a graph.

The paper reads as follows. In the next section, we provide all the important definitions related to the (edge-)Hosoya polynomial and corresponding topological indices. In Section 3, we prove some preliminary results related to certain sets of vertices and edges which are also used in the definitions of Szeged-like topological indices. The main result is then developed in Section 4. In particular, we provide a formula for calculating the edge-Hosoya polynomial of a graph G obtained from connected bipartite graphs G_1 and G_2 by identifying two edges. Finally, in Section 5 we show how the main theorem can be applied to phenylene chains. Therefore, the recurrence relations for computing the edge-Hosoya polynomial of these graphs are provided and an algorithm is presented that calculates the polynomial of any phenylene chain in linear time with respect to the number of hexagons. In addition, closed formula for the edge-Hosoya polynomial of linear phenylene chains is obtained and consequently, the edge-Wiener index and the edge-hyper-Wiener index of the mentioned graphs are recalculated.

2 The (edge-)Hosoya polynomial and related indices

Let $G = (V(G), E(G))$ be a connected graph. We denote by $d_G(x, y)$ the usual shortest path distance between vertices x and y of a graph G and by $\deg(x)$ the degree of x. The distance between a vertex x and an edge $e = uv$ is defined as $d_G(x, e) = \min\{d_G(x, u), d_G(x, v)\}$.

One way to define the "distance" between edges $e = ab$ and $f = uv$ of a graph G is the following:

$$\widehat{d}_G(e, f) = \min\{d_G(a, u), d_G(a, v), d_G(b, u), d_G(b, v)\}\,.$$

However, the pair $(E(G), \widehat{d}_G)$ is not a metric space since distinct edges may have distance zero. Therefore, the distance $d_G(e, f)$ between edges e and f is defined as the distance between vertices e and f in the line graph $L(G)$ [12]. There is a simple relation between $\widehat{d}_G$ and d_G, since $d_G(e, f) = \widehat{d}_G(e, f) + 1$ if $e \neq f$ and $d_G(e, f) = \widehat{d}_G(e, f) = 0$ if $e = f$.

Next, we formally define the Hosoya and the edge-Hosoya polynomials. If G is a connected graph and if $d_v(G, k)$ is the number of (unordered) pairs of its vertices that are at distance k, then the *Hosoya polynomial* of G is

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

The Hosoya polynomial can be also written as

$$H(G,x) = \sum_{\{u,v\} \subseteq V(G)} x^{d_G(u,v)}.$$

Let G be a connected graph with m edges. If $d_e(G,k)$ is the number of (unordered) pairs of its edges that are at distance k, then the *edge-Hosoya polynomial* of G is

$$H_e(G,x) = \sum_{k \geq 0} d_e(G,k)\, x^k = \sum_{\{e,f\} \subseteq E(G)} x^{d_G(e,f)}.$$

Note that $d_e(G,0) = m$ and that the following relation holds for any connected graph G:

$$H_e(G,x) = H(L(G),x).$$

As already mentioned, the defined polynomials are important because they are closely related to the (edge-)Wiener index. To state the connection, we first define the *Wiener index* $W(G)$ and the *edge-Wiener index* $W_e(G)$ of a connected graph G:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v), \quad W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d_G(e,f).$$

It is easy to see that the following formulas hold true:

$$W(G) = H'(G,1), \quad W_e(G) = H'_e(G,1).$$

On the other hand, the *edge-hyper-Wiener index* of a connected graph G is defined as

$$WW_e(G) = \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d_G(e,f) + \frac{1}{2} \sum_{\{e,f\} \subseteq E(G)} d_G(e,f)^2$$

and the following connection to the edge-Hosoya polynomial was proved in [21]:

$$WW_e(G) = H'_e(G,1) + \frac{1}{2}H''_e(G,1). \tag{1}$$

Finally, we add some definitions that will be used later. If G is a graph, $k \geq 0$ an integer, and $v \in V(G)$ a vertex, then $d_e(G,v,k)$ is the number of edges of G at distance k from v. Obviously, $d_e(G,v,0) = \deg(v)$. The polynomial $H_e(G,v,x)$ is defined as

$$H_e(G,v,x) = \sum_{k\geq 0} d_e(G,v,k)x^k = \sum_{e\in E(G)} x^{d_G(v,e)}.$$

If G is a graph, $k \geq 0$ an integer, and $e \in E(G)$ an edge, then $d_e(G,e,k)$ is the number of edges of G at distance k from e. It is obvious that $d(G,e,0) = 1$. The polynomial $H_e(G,e,x)$ is defined in the following way:

$$H_e(G,e,x) = \sum_{k\geq 0} d_e(G,e,k)x^k = \sum_{f\in E(G)} x^{d_G(f,e)}.$$

3 Preliminary results

In this short section, we introduce some notation which is usually used to define various Szeged-like topological indices [5], but will be needed later to state the main result of this paper. Moreover, two related lemmas are proved.

Let G be a connected graph and let $e = uv$ be an edge of G. The following notation for the sets of vertices and edges of G will be used:

$$\begin{aligned}
N_u(e|G) &= \{x \in V(G) \mid d_G(x,u) < d_G(x,v)\},\\
N_v(e|G) &= \{x \in V(G) \mid d_G(x,v) < d_G(x,u)\},\\
N_0(e|G) &= \{x \in V(G) \mid d_G(x,u) = d_G(x,v)\},\\
M_u(e|G) &= \{f \in E(G) \mid d_G(f,u) < d_G(f,v)\},\\
M_v(e|G) &= \{f \in E(G) \mid d_G(f,v) < d_G(f,u)\},\\
M_0(e|G) &= \{f \in E(G) \mid d_G(f,u) = d_G(f,v)\}.
\end{aligned}$$

It is worth mentioning that if G is a bipartite graph, the set $N_0(e|G)$ is always empty.

Next, we state and prove two lemmas that will be needed in Section 4.

Lemma 3.1. *Let G be a connected graph, and let $e = uv$ and $f = ab$ be two edges of G. If $a \in N_u(e|G)$ and $b \in N_v(e|G)$, then*

$$d_G(a,u) = d_G(b,v) = d_G(a,v) - 1 = d_G(b,u) - 1.$$

Proof. By assumption we have $d_G(a,u) < d_G(a,v)$ and $d_G(b,v) < d_G(b,u)$. Let us denote $d_G(a,u) = k$ and $d_G(b,v) = \ell$. Then $d_G(a,v) = k+1$ and $d_G(b,u) = \ell+1$. On the other hand, there is a path of length $\ell+1$ between a and v, which means $d_G(a,v) \leq \ell+1$. Therefore $k \leq \ell$. Similarly, there is a path of length $k+1$ between b and u, which means $d_G(b,u) \leq k+1$. Therefore $\ell \leq k$, and consequently $k = \ell$. ■

The following lemma shows another way to define the sets $M_u(e|G)$, $M_v(e|G)$, and $M_0(e|G)$ in bipartite graphs.

Lemma 3.2. *If G is a connected bipartite graph and $e = uv \in E(G)$, then*

$$\begin{aligned} M_u(e|G) &= \{f = ab \in E(G) \mid a \in N_u(e|G) \ \wedge \ b \in N_u(e|G)\}, \\ M_v(e|G) &= \{f = ab \in E(G) \mid a \in N_v(e|G) \ \wedge \ b \in N_v(e|G)\}, \\ M_0(e|G) &= \{f = ab \in E(G) \mid (a \in N_u(e|G) \ \wedge \ b \in N_v(e|G)) \ \vee \\ &\qquad (a \in N_v(e|G) \ \wedge \ b \in N_u(e|G))\}. \end{aligned}$$

Proof. We set the following notation:

$$\begin{aligned} A &= \{f = ab \in E(G) \mid a \in N_u(e|G) \ \wedge \ b \in N_u(e|G)\}, \\ B &= \{f = ab \in E(G) \mid a \in N_v(e|G) \ \wedge \ b \in N_v(e|G)\}, \\ C &= \{f = ab \in E(G) \mid (a \in N_u(e|G) \ \wedge \ b \in N_v(e|G)) \ \vee \\ &\qquad (a \in N_v(e|G) \ \wedge \ b \in N_u(e|G))\}. \end{aligned}$$

If $f = ab \in A$, then $d_G(a,u) < d_G(a,v)$ and $d_G(b,u) < d_G(b,v)$ and hence

$$d_G(f,u) = \min\{d_G(a,u), d_G(b,u)\} < \min\{d_G(a,v), d_G(b,v)\} = d_G(f,v).$$

This means $f \in M_u(e|G)$ and consequently $A \subseteq M_u(e|G)$. In a similar way we can show $B \subseteq M_v(e|G)$. Next, let $f = ab \in C$ and without loss of generality suppose that $a \in N_u(e|G)$ and $b \in N_v(e|G)$. By Lemma 3.1 it follows $d_G(a,u) = d_G(b,v)$ and $d_G(a,v) = d_G(b,u) = d_G(a,u) + 1 = d_G(b,v) + 1$. Therefore,

$$d_G(f,u) = d_G(a,u) = d_G(b,v) = d_G(f,v),$$

which implies $f \in M_0(e|G)$. As a result, we have $C \subseteq M_0(e|G)$.

Since $E(G) = A \cup B \cup C = M_u(e|G) \cup M_v(e|G) \cup M_0(e|G)$ and also $A \subseteq M_u(e|G)$, $B \subseteq M_v(e|G)$, $C \subseteq M_0(e|G)$, we conclude

$$A = M_u(e|G), \quad B = M_v(e|G), \quad \text{and} \quad C = M_0(e|G). \qquad \blacksquare$$

4 A method for computing the edge-Hosoya polynomial by identifying two edges

In this section, we present a new method for computing the edge-Hosoya polynomial of a graph by using edge-Hosoya polynomials of its subgraphs. In particular, we describe how the edge-Hosoya polynomials of graphs G_1 and G_2 can be used to compute the edge-Hosoya polynomial of a graph G obtained by identifying two edges. The stated result will be applied in the next section, where we consider phenylene chains.

Let G_1 and G_2 be two connected bipartite graphs and let $e_1 \in E(G_1)$, $e_2 \in E(G_2)$. The graph G is obtained from G_1 and G_2 by identifying edges e_1 and e_2 into an edge $e' = uv$, see Figure 1.

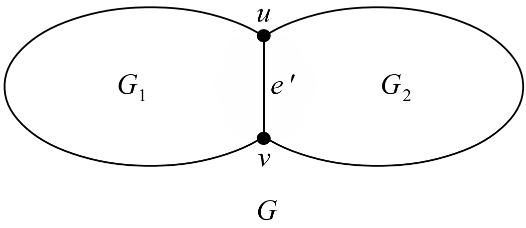

Figure 1. A graph G obtained from graphs G_1 and G_2 by identifying edges $e_1 \in E(G_1)$ and $e_2 \in E(G_2)$ into an edge $e' = uv$.

In the following, we write e' instead of e_1 or e_2. Moreover, for $i \in \{1, 2\}$ we use the following notation:

$$E_u(G_i) = M_u(e'|G_i), \quad E_v(G_i) = M_v(e'|G_i), \quad \text{and} \quad E_0(G_i) = M_0(e'|G_i).$$

We start with one simple observation and several lemmas.

Observation 4.1. *Let $i \in \{1, 2\}$. If $x, y \in V(G_i)$ and $e, f \in E(G_i)$, then*

$$d_G(x, y) = d_{G_i}(x, y) \quad \textit{and} \quad d_G(e, f) = d_{G_i}(e, f).$$

To prove the following lemmas, we consider different cases according to Lemma 3.2.

Lemma 4.2. *Let $f \in E(G_1)$. If $e \in E_u(G_2) \setminus \{e'\}$, then*

$$d_G(e, f) = d_{G_2}(e, u) + d_{G_1}(u, f) + 1.$$

Similarly, if $e \in E_v(G_2) \setminus \{e'\}$, then

$$d_G(e, f) = d_{G_2}(e, v) + d_{G_1}(v, f) + 1.$$

Proof. We prove only the first part, since the second is analogous.

Let $e = ab$ and $f = xy$. Also, without loss of generality suppose $d_{G_2}(a, u) < d_{G_2}(b, u)$, which means $d_{G_2}(e, u) = d_{G_2}(a, u)$. We consider three cases:

Case 1: $f \in E_u(G_1)$. Without loss of generality assume $d_{G_1}(x, u) < d_{G_1}(y, u)$. Then $d_{G_1}(u, f) = d_{G_1}(u, x)$ and since any shortest path from a

to x goes through u, we also have

$$d_G(a,x) = d_{G_2}(a,u) + d_{G_1}(u,x) \quad \text{and} \quad \widehat{d}_G(e,f) = d_G(a,x).$$

Since $e \neq f$, we have

$$d_G(e,f) = \widehat{d}_G(e,f) + 1 = d_{G_2}(a,u) + d_{G_1}(u,x) + 1 = d_{G_2}(e,u) + d_{G_1}(u,f) + 1.$$

Case 2: $f \in E_v(G_1)$. Without loss of generality assume $d_{G_1}(x,v) < d_{G_1}(y,v)$. Then $d_{G_1}(v,f) = d_{G_1}(v,x)$ and consequently it holds $d_{G_1}(u,f) = d_{G_1}(u,x) = 1 + d_{G_1}(v,x)$. Since there exists a shortest path from a to x that goes through u and v, we have

$$d_G(a,x) = d_{G_2}(a,u) + 1 + d_{G_1}(v,x) = d_{G_2}(a,u) + d_{G_1}(u,x)$$

and $\widehat{d}_G(e,f) = d_G(a,x)$. Hence,

$$d_G(e,f) = d_G(a,x) + 1 = d_{G_2}(a,u) + d_{G_1}(u,x) + 1 = d_{G_2}(e,u) + d_{G_1}(u,f) + 1.$$

Case 3: $f \in E_0(G_1)$. Without loss of generality assume $d_{G_1}(x,u) < d_{G_1}(x,v)$, $d_{G_1}(y,v) < d_{G_1}(y,u)$. Then $d_{G_1}(u,f) = d_{G_1}(u,x)$ and by Lemma 3.1, $d_{G_1}(u,x) = d_{G_1}(v,y)$. Since any shortest path from a to x goes through u, we can use the same reasoning as in Case 1. ■

Lemma 4.3. *If* $e \in E_0(G_2) \setminus \{e'\}$ *and* $f \in E(G_1) \setminus \{e'\}$, *then*

$$d_G(e,f) = d_{G_2}(e,e') + d_{G_1}(e',f) - 1.$$

Proof. Let $e = ab$ and $f = xy$. Without loss of generality assume that $d_{G_2}(a,u) < d_{G_2}(a,v)$, $d_{G_2}(b,v) < d_{G_2}(b,u)$, which means $d_{G_2}(a,u) = d_{G_2}(b,v)$ and $\widehat{d}_{G_2}(e,e') = d_{G_2}(a,u)$. We consider three cases:

Case 1: $f \in E_u(G_1)$. Assume that $d_{G_1}(x,u) < d_{G_1}(y,u)$. Then $\widehat{d}_{G_1}(e',f) = d_{G_1}(u,x)$ and since any shortest path from a to x goes through u, we also have

$$d_G(a,x) = d_{G_2}(a,u) + d_{G_1}(u,x) \quad \text{and} \quad \widehat{d}_G(e,f) = d_G(a,x).$$

Hence,

$$\begin{aligned} d_G(e,f) &= d_G(a,x)+1 = d_{G_2}(a,u)+d_{G_1}(u,x)+1 \\ &= (d_{G_2}(e,e')-1)+(d_{G_1}(e',f)-1)+1 \\ &= d_{G_2}(e,e')+d_{G_1}(e',f)-1. \end{aligned}$$

Case 2: $f \in E_v(G_1)$. Due to symmetry, this case is analogous to Case 1.

Case 3: $f \in E_0(G_1)$. We may assume $d_{G_1}(x,u) < d_{G_1}(x,v)$ and $d_{G_1}(y,v) < d_{G_1}(y,u)$. By Lemma 3.1, $\widehat{d}_{G_1}(e',f) = d_{G_1}(u,x) = d_{G_1}(v,y)$. Since any shortest path from a to x goes through u, we can use the same reasoning as in Case 1. ■

Lemma 4.4. *Let $f \in E(G_1)$. If $a \in N_u(e'|G_2)$, then*

$$d_G(a,f) = d_{G_2}(a,u) + d_{G_1}(u,f).$$

Similarly, if $a \in N_v(e'|G_2)$, then

$$d_G(a,f) = d_{G_2}(a,v) + d_{G_1}(v,f).$$

Proof. We prove only the first part, since the second can be shown in a similar way. Suppose $a \in N_u(e'|G_2)$, $f = xy$ and consider the following three cases:

Case 1: $f \in E_u(G_1)$. Without loss of generality assume $d_{G_1}(x,u) < d_{G_1}(y,u)$. Therefore, $d_{G_1}(u,f) = d_{G_1}(u,x)$ and since any shortest path from a to x goes through u, we also have

$$d_G(a,x) = d_{G_2}(a,u) + d_{G_1}(u,x) \quad \text{and} \quad d_G(a,f) = d_G(a,x).$$

Hence,

$$d_G(a,f) = d_G(a,x) = d_{G_2}(a,u) + d_{G_1}(u,x) = d_{G_2}(a,u) + d_{G_1}(u,f).$$

Case 2: $f \in E_v(G_1)$. Without loss of generality assume $d_{G_1}(x,v) < d_{G_1}(y,v)$. Therefore, $d_{G_1}(v,f) = d_{G_1}(v,x)$ and consequently $d_{G_1}(u,f) =$

$d_{G_1}(u,x) = 1 + d_{G_1}(v,x)$. Since there exists a shortest path from a to x that goes through u and v, we have

$$d_G(a,x) = d_{G_2}(a,u) + 1 + d_{G_1}(v,x) = d_{G_2}(a,u) + d_{G_1}(u,x)$$

and $d_G(a,f) = d_G(a,x)$. Hence,

$$d_G(a,f) = d_G(a,x) = d_{G_2}(a,u) + d_{G_1}(u,x) = d_{G_2}(a,u) + d_{G_1}(u,f).$$

Case 3: $f \in E_0(G_1)$. Without loss of generality assume $d_{G_1}(x,u) < d_{G_1}(x,v)$, $d_{G_1}(y,v) < d_{G_1}(y,u)$. Hence, $d_{G_1}(u,f) = d_{G_1}(u,x)$ and by Lemma 3.1, $d_{G_1}(u,x) = d_{G_1}(v,y)$. Since any shortest path from a to x goes through u, we can use the same reasoning as in Case 1. ■

The main result of the paper can now be stated.

Theorem 4.5. *Let G be a graph obtained from connected bipartite graphs G_1 and G_2 by identifying the edges $e_1 \in E(G_1)$ and $e_2 \in E(G_2)$ into an edge $e' = uv$. Then*

$$\begin{aligned} H_e(G,x) &= H_e(G_1,x) + H_e(G_2,x) - H_e(G_2,e',x) \\ &+ \sum_{e \in E_u(G_2)} x^{d_{G_2}(e,u)+1} H_e(G_1,u,x) \\ &+ \sum_{e \in E_v(G_2)} x^{d_{G_2}(e,v)+1} H_e(G_1,v,x) \\ &+ \sum_{e \in E_0(G_2)\setminus\{e'\}} x^{d_{G_2}(e,e')-1} H_e(G_1,e',x) \\ &+ \sum_{e \in E_0(G_2)\setminus\{e'\}} (x-1)x^{d_{G_2}(e,e')-1}. \end{aligned}$$

Proof. Obviously, the edge-Hosoya polynomial can be written as the sum of the following contributions:

$$\begin{aligned} H_e(G,x) &= \sum_{\{e,f\} \subseteq E(G_1)} x^{d_G(e,f)} + \sum_{\{e,f\} \subseteq E(G_2)} x^{d_G(e,f)} \\ &- x^{d_G(e',e')} + \sum_{e \in E(G_2)\setminus\{e'\}} \sum_{f \in E(G_1)\setminus\{e'\}} x^{d_G(e,f)}, \end{aligned}$$

where the third term on the right-hand side is needed since the pair $\{e', e'\}$ is counted in the first and also in the second sum. By Observation 4.1 we obtain

$$\sum_{\{e,f\}\subseteq E(G_1)} x^{d_G(e,f)} = H_e(G_1, x) \quad \text{and} \quad \sum_{\{e,f\}\subseteq E(G_2)} x^{d_G(e,f)} = H_e(G_2, x).$$

Next, we observe that

$$\begin{aligned}
&\sum_{e\in E(G_2)\setminus\{e'\}} \sum_{f\in E(G_1)\setminus\{e'\}} x^{d_G(e,f)} \\
&\qquad = \sum_{e\in E(G_2)\setminus\{e'\}} \left(x^{d_G(e,e')} + \sum_{f\in E(G_1)\setminus\{e'\}} x^{d_G(e,f)} \right) \\
&\qquad - \sum_{e\in E(G_2)\setminus\{e'\}} x^{d_G(e,e')} \\
&\qquad = \sum_{e\in E(G_2)\setminus\{e'\}} \sum_{f\in E(G_1)} x^{d_G(e,f)} - (H_e(G_2, e', x) - 1)
\end{aligned}$$

and therefore deduce the following formula:

$$\begin{aligned}
H_e(G, x) &= H_e(G_1, x) + H_e(G_2, x) - H_e(G, e', x) \\
&\quad + \sum_{e\in E(G_2)\setminus\{e'\}} \sum_{f\in E(G_1)} x^{d_G(e,f)}.
\end{aligned} \tag{2}$$

Finally, we analyse the last term of the previous equation. Firstly, we partition it into three sums:

$$\begin{aligned}
\sum_{e\in E(G_2)\setminus\{e'\}} \sum_{f\in E(G_1)} x^{d_G(e,f)} &= \sum_{e\in E_u(G_2)} \sum_{f\in E(G_1)} x^{d_G(e,f)} \\
&\quad + \sum_{e\in E_v(G_2)} \sum_{f\in E(G_1)} x^{d_G(e,f)} \\
&\quad + \sum_{e\in E_0(G_2)\setminus\{e'\}} \sum_{f\in E(G_1)} x^{d_G(e,f)}.
\end{aligned} \tag{3}$$

To complete the proof, we separately consider each of the three sums on the right-hand side of the previous equation. By using the first part of

Lemma 4.2, we have

$$\begin{aligned}\sum_{e\in E_u(G_2)}\sum_{f\in E(G_1)} x^{d_G(e,f)} &= \sum_{e\in E_u(G_2)}\sum_{f\in E(G_1)} x^{d_{G_2}(e,u)+1+d_{G_1}(u,f)}\\ &= \sum_{e\in E_u(G_2)} x^{d_{G_2}(e,u)+1}\sum_{f\in E(G_1)} x^{d_{G_1}(u,f)}\\ &= \sum_{e\in E_u(G_2)} x^{d_{G_2}(e,u)+1}H_e(G_1,u,x).\end{aligned}$$

Similarly, by the second part of Lemma 4.2 one can get

$$\sum_{e\in E_v(G_2)}\sum_{f\in E(G_1)} x^{d_G(e,f)} = \sum_{e\in E_v(G_2)} x^{d_{G_2}(e,v)+1}H_e(G_1,v,x).$$

Moreover, we analyse the third sum and apply Lemma 4.3:

$$\begin{aligned}&\sum_{e\in E_0(G_2)\setminus\{e'\}}\sum_{f\in E(G_1)} x^{d_G(e,f)}\\ &= \sum_{e\in E_0(G_2)\setminus\{e'\}}\left(x^{d_G(e,e')}+\sum_{f\in E(G_1)\setminus\{e'\}} x^{d_G(e,f)}\right)\\ &= \sum_{e\in E_0(G_2)\setminus\{e'\}}\left(x^{d_G(e,e')}+\sum_{f\in E(G_1)\setminus\{e'\}} x^{d_G(e,e')+d_G(e',f)-1}\right)\\ &= \sum_{e\in E_0(G_2)\setminus\{e'\}}\left(x^{d_{G_2}(e,e')}+x^{d_{G_2}(e,e')-1}\sum_{f\in E(G_1)\setminus\{e'\}} x^{d_{G_1}(e',f)}\right)\\ &= \sum_{e\in E_0(G_2)\setminus\{e'\}}\left(x^{d_{G_2}(e,e')}+x^{d_{G_2}(e,e')-1}\left(H_e(G_1,e',x)-1\right)\right)\\ &= \sum_{e\in E_0(G_2)\setminus\{e'\}} x^{d_{G_2}(e,e')-1}H_e(G_1,e',x)\\ &+ \sum_{e\in E_0(G_2)\setminus\{e'\}} (x-1)x^{d_{G_2}(e,e')-1}.\end{aligned}$$

By taking the last three equations in (3) and consequently in (2), we obtain the desired result. ■

5 Application to phenylenes

In this section, we apply Theorem 4.5 to an important family of molecular graphs called phenylenes. Firstly, some definitions are needed.

A *benzenoid graph* is a simple bipartite 2-connected plane graph with all internal vertices of degree 3 and all boundary vertices of degree 2 or 3 such that the boundary of any inner face is a 6-cycle. Inner faces of a benzenoid graph are simply called *hexagons.* Moreover, a benzenoid graph is said to be *catacondensed* if it does not possess internal vertices.

Let B be a catacondensed benzenoid graph with at least two hexagons. If we add *quadrilaterals* (faces whose boundary is a 4-cycle) between all pairs of adjacent hexagons of B, the obtained graph G is called a *phenylene*, see Figure 2.

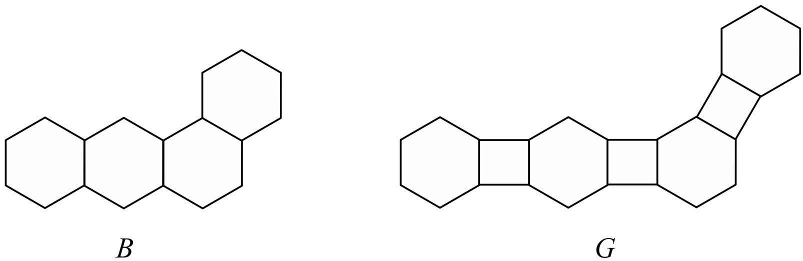

Figure 2. A benzenoid graph B and the corresponding phenylene G.

A hexagon of a phenylene G is called *branched* if it is adjacent to exactly three other inner faces of G. Moreover, a phenylene which does not contain a branched hexagon is called a *phenylene chain.* In Figure 2 we can see a phenylene chain with four hexagons. Furthermore, a graph obtained from a quadrilateral and a hexagon by identifying two edges will be referred to as a *basic compound* of a phenylene.

5.1 Adding a basic compound of a phenylene

In this subsection we apply Theorem 4.5 to calculate the edge-Hosoya polynomial of a graph obtained by adding the basic compound of a phenylene to another graph. Therefore, let G be a graph obtained by identifying two edges of a connected bipartite graph G_1 and the basic compound of a phenylene, see Figure 3.

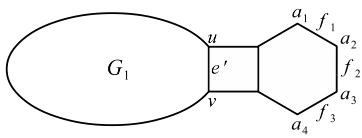

Figure 3. A graph G obtained from G_1 and the basic compound of a phenylene.

We obtain the following corollary.

Corollary 5.1. *If G is a graph obtained from a connected bipartite graph G_1 and the basic compound of a phenylene by identifying two edges into an edge $e' = uv$ as shown in Figure 3, then*

$$\begin{aligned} H_e(G,x) &= H_e(G_1,x) + (x+x^2+x^3)H_e(G_1,u,x) \\ &+ (x+x^2+x^3)H_e(G_1,v,x) + (x+x^3)H_e(G_1,e',x) \\ &+ 8+9x+12x^2+6x^3+x^4. \end{aligned}$$

Proof. Denote by G_2 the basic compound of a phenylene. Then it is easy to see that

$$\begin{aligned} H_e(G_2,x) &= 9+12x+14x^2+9x^3+x^4, \\ H_e(G_2,e',x) &= 1+2x+3x^2+2x^3+x^4, \\ \sum_{e\in E_u(G_2)} x^{d_{G_2}(e,u)+1} H_e(G_1,u,x) &= (x+x^2+x^3)H_e(G_1,u,x), \\ \sum_{e\in E_v(G_2)} x^{d_{G_2}(e,v)+1} H_e(G_1,v,x) &= (x+x^2+x^3)H_e(G_1,v,x), \\ \sum_{e\in E_0(G_2)\setminus\{e'\}} x^{d_{G_2}(e,e')-1} H_e(G_1,e',x) &= (x+x^3)H_e(G_1,e',x), \\ \sum_{e\in E_0(G_2)\setminus\{e'\}} (x-1)x^{d_{G_2}(e,e')-1} &= x^2+x^4-x-x^3. \end{aligned}$$

By taking all six equations stated above into the formula of Theorem 4.5, we obtain the desired result. ∎

In the following proposition we describe how the edge-Hosoya polynomials of G with a fixed vertex or an edge can be obtained from a smaller graph G_1. The specific shape of the polynomial depends on the exact position on which the basic compound of a phenylene was attached, and this yields specific forms of partial polynomials.

Proposition 5.2. *Let all the notation be as in Figure 3. Then*

1. $H_e(G, a_1, x) = x^2 H_e(G_1, u, x) + 2 + 3x + 3x^2$,
2. $H_e(G, a_2, x) = x^3 H_e(G_1, u, x) + 2 + 2x + 3x^2 + x^3$,
3. $H_e(G, a_3, x) = x^3 H_e(G_1, v, x) + 2 + 2x + 3x^2 + x^3$,
4. $H_e(G, a_4, x) = x^2 H_e(G_1, v, x) + 2 + 3x + 3x^2$,
5. $H_e(G, f_1, x) = x^3 H_e(G_1, u, x) + 1 + 2x + 3x^2 + 2x^3$,
6. $H_e(G, f_2, x) = x^3 H_e(G_1, e', x) + 1 + 2x + 2x^2 + 2x^3 + x^4$,
7. $H_e(G, f_3, x) = x^3 H_e(G_1, v, x) + 1 + 2x + 3x^2 + 2x^3$.

Proof. We include the proofs of formulas 1., 5., and 6. The remaining formulas can be proved in a analogous way.

1. By using Lemma 4.4 in the third equality, we obtain

$$\begin{aligned} H_e(G, a_1, x) &= \sum_{f \in E(G)} x^{d_G(a_1, f)} \\ &= \sum_{f \in E(G_1)} x^{d_G(a_1, f)} + \sum_{f \in E(G_2) \setminus \{e'\}} x^{d_G(a_1, f)} \\ &= \sum_{f \in E(G_1)} x^{d_{G_2}(a_1, u) + d_{G_1}(u, f)} + \sum_{f \in E(G_2) \setminus \{e'\}} x^{d_G(a_1, f)} \\ &= \sum_{f \in E(G_1)} x^{d_{G_1}(u, f) + 2} + \sum_{f \in E(G_2) \setminus \{e'\}} x^{d_{G_2}(a_1, f)} \\ &= x^2 \sum_{f \in E(G_1)} x^{d_{G_1}(u, f)} + 2 + 3x + 3x^2 \\ &= x^2 H_e(G_1, u, x) + 2 + 3x + 3x^2. \end{aligned}$$

5. By applying Lemma 4.2 in the third equality, one can get

$$\begin{aligned}
H_e(G, f_1, x) &= \sum_{f \in E(G)} x^{d_G(f, f_1)} \\
&= \sum_{f \in E(G_1)} x^{d_G(f, f_1)} + \sum_{f \in E(G_2) \setminus \{e'\}} x^{d_G(f, f_1)} \\
&= \sum_{f \in E(G_1)} x^{d_{G_1}(f, u) + d_{G_2}(u, f_1) + 1} + \sum_{f \in E(G_2) \setminus \{e'\}} x^{d_G(f, f_1)} \\
&= \sum_{f \in E(G_1)} x^{d_{G_1}(f, u) + 3} + \sum_{f \in E(G_2) \setminus \{e'\}} x^{d_{G_2}(f, f_1)} \\
&= x^3 \sum_{f \in E(G_1)} x^{d_{G_1}(f, u)} + 1 + 2x + 3x^2 + 2x^3 \\
&= x^3 H_e(G_1, u, x) + 1 + 2x + 3x^2 + 2x^3.
\end{aligned}$$

6. By using Lemma 4.3 in the third equality, we obtain

$$\begin{aligned}
H_e(G, f_2, x) &= \sum_{f \in E(G)} x^{d_G(f, f_2)} \\
&= \sum_{f \in E(G_1) \setminus \{e'\}} x^{d_G(f, f_2)} + x^4 + \sum_{f \in E(G_2) \setminus \{e'\}} x^{d_G(f, f_2)} \\
&= \sum_{f \in E(G_1) \setminus \{e'\}} x^{d_{G_2}(f_2, e') + d_{G_1}(e', f) - 1} + x^4 \\
&+ \sum_{f \in E(G_2) \setminus \{e'\}} x^{d_{G_2}(f, f_2)} \\
&= \sum_{f \in E(G_1) \setminus \{e'\}} x^{3 + d_{G_1}(e', f)} + x^4 + (1 + 2x + 2x^2 + 3x^3) \\
&= x^3 \left(\sum_{f \in E(G_1) \setminus \{e'\}} x^{d_{G_1}(e', f)} + 1 - 1 \right) \\
&+ 1 + 2x + 2x^2 + 3x^3 + x^4 \\
&= x^3 \sum_{f \in E(G_1)} x^{d_{G_1}(e', f)} - x^3 + 1 + 2x + 2x^2 + 3x^3 + x^4 \\
&= x^3 H_e(G_1, e', x) + 1 + 2x + 2x^2 + 2x^3 + x^4.
\end{aligned}$$

■

5.2 Recurrence relations for phenylene chains

Here we use Corollary 5.1 and Proposition 5.2 to recursively calculate the edge-Hosoya polynomial of any phenylene chain.

Therefore, let Ph_1 be a hexagon. Moreover, for $r > 1$ we denote by Ph_r a phenylene chain with exactly r hexagons obtained from Ph_{r-1} by adding the basic compound of a phenylene over the edge $e_{r-1} = u_{r-1}v_{r-1}$. If $r > 1$, by Corollary 5.1 we have

$$\begin{aligned} H_e(Ph_r, x) &= H_e(Ph_{r-1}, x) + (x + x^3)H_e(Ph_{r-1}, e_{r-1}, x) \\ &+ (x + x^2 + x^3)\left(H_e(Ph_{r-1}, u_{r-1}, x) + H_e(Ph_{r-1}, v_{r-1}, x)\right) \\ &+ 8 + 9x + 12x^2 + 6x^3 + x^4. \end{aligned}$$

In accordance with the notation described above, $e_r = u_r v_r$ is the edge that is used to obtain Ph_{r+1} from Ph_r. There are three possibilities for this edge, see Figure 4.

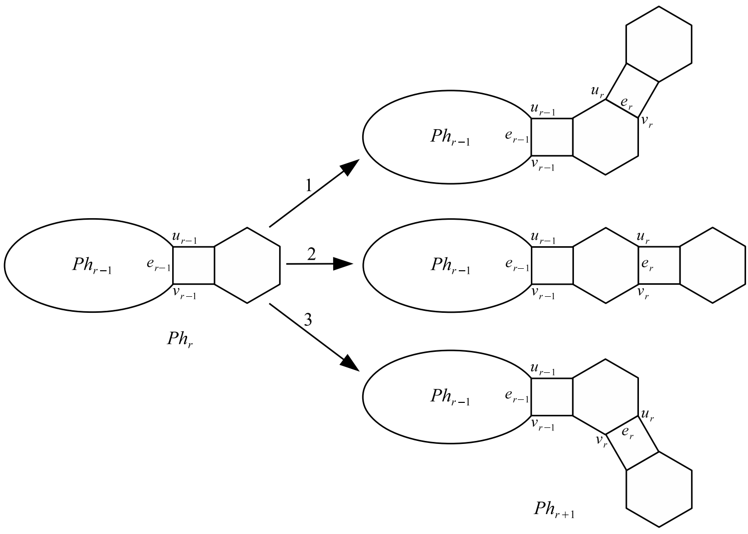

Figure 4. Three possible cases for adding the basic compound of a phenylene to Ph_r.

For these cases, Proposition 5.2 gives the following formulas.

Case 1:

$$\begin{aligned} H_e(Ph_r, u_r, x) &= x^2 H_e(Ph_{r-1}, u_{r-1}, x) + 2 + 3x + 3x^2, \\ H_e(Ph_r, v_r, x) &= x^3 H_e(Ph_{r-1}, u_{r-1}, x) + 2 + 2x + 3x^2 + x^3, \\ H_e(Ph_r, e_r, x) &= x^3 H_e(Ph_{r-1}, u_{r-1}, x) + 1 + 2x + 3x^2 + 2x^3. \end{aligned}$$

Case 2:

$$\begin{aligned} H_e(Ph_r, u_r, x) &= x^3 H_e(Ph_{r-1}, u_{r-1}, x) + 2 + 2x + 3x^2 + x^3, \\ H_e(Ph_r, v_r, x) &= x^3 H_e(Ph_{r-1}, v_{r-1}, x) + 2 + 2x + 3x^2 + x^3, \\ H_e(Ph_r, e_r, x) &= x^3 H_e(Ph_{r-1}, e_{r-1}, x) + 1 + 2x + 2x^2 + 2x^3 + x^4. \end{aligned}$$

Case 3:

$$\begin{aligned} H_e(Ph_r, u_r, x) &= x^3 H_e(Ph_{r-1}, v_{r-1}, x) + 2 + 2x + 3x^2 + x^3, \\ H_e(Ph_r, v_r, x) &= x^2 H_e(Ph_{r-1}, v_{r-1}, x) + 2 + 3x + 3x^2, \\ H_e(Ph_r, e_r, x) &= x^3 H_e(Ph_{r-1}, v_{r-1}, x) + 1 + 2x + 3x^2 + 2x^3. \end{aligned}$$

To present the recursive relations in a more compact way, we use the following notation: $\alpha_r \equiv H_e(Ph_r, x)$, $\beta_r \equiv H_e(Ph_r, u_r, x)$, $\gamma_r \equiv H_e(Ph_r, v_r, x)$, and $\delta_r \equiv H_e(Ph_r, e_r, x)$.
By applying the equations stated above, we immediately obtain the next theorem.

Theorem 5.3. *Let Ph_r be a phenylene chain with r hexagons. If $r = 1$, we have*

$$\alpha_1 = 6+6x+6x^2+3x^3, \quad \beta_1 = \gamma_1 = 2+2x+2x^2, \quad \delta_1 = 1+2x+2x^2+x^3.$$

Moreover, for $r > 1$ it holds

$$\alpha_r = \alpha_{r-1}+(x+x^2+x^3)(\beta_{r-1}+\gamma_{r-1})+(x+x^3)\delta_{r-1}+8+9x+12x^2+6x^3+x^4.$$

In addition, β_r, γ_r, and δ_r satisfy the following recurrences with respect to the cases shown in Figure 4:

Case 1: $\beta_r = x^2\beta_{r-1} + 2 + 3x + 3x^2$, $\gamma_r = x^3\beta_{r-1} + 2 + 2x + 3x^2 + x^3$, $\delta_r = x^3\beta_{r-1} + 1 + 2x + 3x^2 + 2x^3$.
Case 2: $\beta_r = x^3\beta_{r-1}+2+2x+3x^2+x^3$, $\gamma_r = x^3\gamma_{r-1}+2+2x+3x^2+x^3$, $\delta_r = x^3\delta_{r-1} + 1 + 2x + 2x^2 + 2x^3 + x^4$.
Case 3: $\beta_r = x^3\gamma_{r-1} + 2 + 2x + 3x^2 + x^3$, $\gamma_r = x^2\gamma_{r-1} + 2 + 3x + 3x^2$, $\delta_r = x^3\gamma_{r-1} + 1 + 2x + 3x^2 + 2x^3$.

Finally, we describe an algorithm that calculates the edge-Hosoya polynomial of any phenylene chain. Some additional notation is need for this purpose.

To a phenylene chain Ph_r with r hexagons we assign the vector of length r, $(s_1, s_2, \ldots, s_r)$, such that $s_1 = s_r = 0$ and if $r > 2$, then for every $i \in \{2, \ldots, r-1\}$ we define $s_i \in \{1, 2, 3\}$ in the following way: if the edge $e_i = u_iv_i$ (which belongs to Ph_i and Ph_{i+1}) corresponds to the Case j in Figure 4, where $j \in \{1, 2, 3\}$, then $s_i = j$. As an example, to the phenylene chain from Figure 2 we assign the vector $(0, 2, 1, 0)$.

By using this notation, we can now present Algorithm 1. For the phenylene chain from Figure 2 the algorithm immediately gives

$$\begin{aligned} H_e(G,x) &= 4x^{11} + 8x^{10} + 17x^9 + 26x^8 + 33x^7 + 43x^6 \\ &+ 50x^5 + 59x^4 + 74x^3 + 73x^2 + 48x + 30. \end{aligned}$$

We conclude the subsection with the following result.

Theorem 5.4. *If Ph_r is a phenylene chain with r hexagons, then Algorithm 1 correctly computes the edge-Hosoya polynomial of Ph_r and can be implemented in $O(r)$ time, in the model where addition and multiplication of polynomials can be performed in constant time.*

Proof. The correctness of the algorithm follows by Theorem 5.3. Since there is only one "for" loop and all the other commands can be implemented in constant time, it is obvious that the time complexity is $O(r)$. ■

5.3 Closed formula for linear phenylene chains

In this final subsection, we show how the results of the paper can be applied to calculate the closed formulas for the edge-Hosoya polynomial of specific

Algorithm 1: The edge-Hosoya polynomial of a phenylene chain

Input: Vector $(s_1, s_2, \ldots, s_r)$ of a phenylene chain Ph_r.

Output: The edge-Hosoya polynomial of Ph_r.

```
ehp := 6 + 6x + 6x^2 + 3x^3
if r = 1 then
    return ehp
end
b0 := 2 + 2x + 2x^2
g0 := 2 + 2x + 2x^2
d0 := 1 + 2x + 2x^2 + x^3
ehp := ehp+(x+x^2+x^3)(b0+g0)+(x+x^3)d0+8+9x+12x^2+6x^3+x^4
if r = 2 then
    return ehp
end
for i = 2, ..., r − 1 do
    if s_i = 1 then
        b := x^2 b0 + 2 + 3x + 3x^2
        g := x^3 b0 + 2 + 2x + 3x^2 + x^3
        d := x^3 b0 + 1 + 2x + 3x^2 + 2x^3
    end
    if s_i = 2 then
        b := x^3 b0 + 2 + 2x + 3x^2 + x^3
        g := x^3 g0 + 2 + 2x + 3x^2 + x^3
        d := x^3 d0 + 1 + 2x + 2x^2 + 2x^3 + x^4
    end
    if s_i = 3 then
        b := x^3 g0 + 2 + 2x + 3x^2 + x^3
        g := x^2 g0 + 2 + 3x + 3x^2
        d := x^3 g0 + 1 + 2x + 3x^2 + 2x^3
    end
    b0 := b,  g0 := g,  d0 := d
    ehp :=
      ehp+(x+x^2+x^3)(b0+g0)+(x+x^3)d0+8+9x+12x^2+6x^3+x^4
end
return ehp
```

types of phenylene chains.

In particular, we focus on linear chains. More precisely, a phenylene chain with r hexagons and corresponding vector $(s_1, s_2, \ldots, s_r)$ is called *linear* if $r \leq 2$ or $r > 2$ and $s_i = 2$ for all $i \in \{2, \ldots, r-1\}$. In the following, the linear phenylene chain with r hexagons will be denoted by PL_r for any $r \geq 1$, see Figure 5.

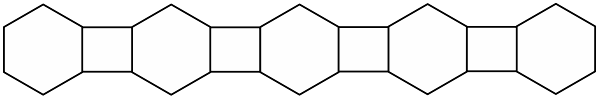

Figure 5. Linear phenylene chain PL_5.

For a linear chain, we always have Case 2 in Theorem 5.3. Therefore, by using the software system SageMath we immediately obtain the closed formulas for β_r, γ_r, and δ_r:

$$\begin{aligned}\beta_r = \gamma_r &= \frac{-x(x^3+3x^2+2x+2)+(2x^3+2x^2+3x+1)x^{3r}}{x(x^3-1)},\\ \delta_r &= \frac{-x(x^3+2x^2+2x+2)+(x^3+2x^2+3x+2)x^{3r}-1}{x^3-1}.\end{aligned}$$

By taking these formulas into the recurrence relation for α_r in Theorem 5.3, we finally get the next result.

Proposition 5.5. *If PL_r is a linear phenylene chain with $r \geq 1$ hexagons, then*

$$\begin{aligned}H_e(PL_r, x) &= \frac{x^{3r}(2+10x+15x^2+18x^3+12x^4+6x^5+x^6)}{(x^3-1)^2}\\ &+ \frac{-(2+8x+16x^2+18x^3+16x^4+4x^5+x^6-2x^7+x^8)}{(x^3-1)^2}\\ &+ \frac{r(8+14x+22x^2+7x^3-6x^4)}{(x^3-1)^2}\\ &+ \frac{r(-23x^5-17x^6-8x^7+x^8+2x^9)}{(x^3-1)^2}.\end{aligned}$$

From the above formula, we can for example get the edge-Hosoya polynomial of phenylene chain PL_5 from Figure 5:

$$\begin{aligned}H_e(PL_5, x) &= x^{15}+6x^{14}+12x^{13}+20x^{12}+27x^{11}+34x^{10}\\ &+ 41x^9+48x^8+56x^7+62x^6+69x^5\\ &+ 78x^4+93x^3+94x^2+62x+38.\end{aligned}$$

Moreover, as a consequence of Proposition 5.5, for linear phenylene chain PL_r, $r \geq 1$, we can calculate the edge-Wiener index,

$$W_e(PL_r) = H'_e(PL_r, 1) = 32r^3 - 7r^2 + 2r, \tag{4}$$

and by using Equation (1) also the edge-hyper-Wiener index,

$$WW_e(PL_r) = 24r^4 + 9r^3 + 2r^2 + 8r - 1. \tag{5}$$

We should mention the edge-Wiener index and the edge-hyper-Wiener index of linear phenylene chains were already calculated in [27] by using the cut method. However, Equation (5) corrects the result from [27], while Equation (4) coincides with the result stated there.

6 Conclusion

In this paper, we proved a formula that can be used to calculate the edge-Hosoya polynomial of a graph G obtained from connected bipartite graphs G_1 and G_2 by identifying two edges. As a consequence, recurrence relations for phenylene chains were derived.

Regarding the future work, it would be interesting to deduce similar methods for computing other distance-based graph polynomials. For example, one could investigate recurrence relations for the Szeged polynomial [1], the edge-Szeged polynomial [3], or the PI polynomial [2].

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