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Generalized Cut Method for Computing Szeged–Like Polynomials with Applications to Polyphenyls and Carbon Nanocones

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Abstract

Szeged, Padmakar-Ivan (PI), and Mostar indices are some of the most investigated distance-based Szeged-like topological indices. On the other hand, the polynomials related to these topological indices were also introduced, for example the Szeged polynomial, the edge-Szeged polynomial, the PI polynomial, the Mostar polynomial, etc. In this paper, we introduce a concept of the general Szeged-like polynomial for a connected strength-weighted graph. It turns out that this concept includes all the above mentioned polynomials and also infinitely many other graph polynomials. As the main result of the paper, we prove a cut method which enables us to efficiently calculate a Szeged-like polynomial by using the corresponding polynomials of strength-weighted quotient graphs obtained by a partition of the edge set that is coarser than Θ^*-partition. To the best of our knowledge, this represents the first implementation of the famous cut method to graph polynomials. Finally, we show how the deduced cut method can be applied to calculate some Szeged-like polynomials and corresponding topological indices of para-polyphenyl chains and carbon nanocones.

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1 Introduction

Topological indices or topological descriptors are numerical parameters of graphs whose purpose is to quantitatively describe various structural properties of the graph topology. When they are used on molecular graphs for the development of quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR), we call them molecular descriptors. On the other hand, topological indices also have numerous other applications in complex networks [20].

One of the oldest molecular descriptors is the well-known Wiener index [43], which is for a connected graph G defined as the sum of distances between all (unordered) pairs of vertices in G. Later, Gutman [25] introduced the *Szeged index*, which is for any connected graph G defined as

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e) n_v(e),$$

where $n_u(e)$ represents the number of vertices of G whose distance to u is smaller than the distance to v and $n_v(e)$ is the number of vertices of G whose distance to v is smaller than the distance to u. Later, the *Padmakar-Ivan (PI) index* was defined [32] with

$$PI(G) = \sum_{e=uv \in E(G)} \big(m_u(e) + m_v(e) \big),$$

where the numbers $m_u(e)$ and $m_v(e)$ are the edge-variants of the numbers $n_u(e)$ and $n_v(e)$. Moreover, the *Mostar index* of G is calculated as

$$Mo(G) = \sum_{e=uv \in E(G)} |n_u(e) - n_v(e)|.$$

Firstly, this index was investigated in [28,40] under the name Co-PI index. However, its current name and notation was proposed in [19].

The Szeged index, the PI index, and the Mostar index are the most known representitatives of the so-called Szeged-like topological indices [15], which include also numerous other topological descriptors, for example the edge-Szeged index [26], weighted Szeged and PI indices [31], weighted

Mostar indices [5], the Graovac-Ghorbani index [24], and the recently introduced Trinajstić index [21]. Especially the Mostar index was intensively investigated in the previous few years, see [1, 13, 17, 30, 44] for some relevant recent papers. It is worth mentioning that besides their applications in chemistry, these indices can be useful also for other purposes, for example to measure network bipartivity [39] or distance-unbalancedness of graphs [37].

In 1988, Hosoya introduced some counting polynomials for chemistry and among them the well-known Hosoya polynomial (also called Wiener polynomial), which is closely related to the Wiener index [29]. Similarly, graph polynomials related to Szeged-like topological indices were also introduced, for example the *Szeged polynomial* $Sz(G,x)$ [9], the *Mostar polynomial* $Mo(G,x)$ [2], the *PI polynomial* $PI(G,x)$ [10], and the *edge-Szeged polynomial* $Sz_e(G,x)$ [11], which are for a connected graph G defined as

$$Sz(G,x) = \sum_{e=uv\in E(G)} x^{n_u(e)n_v(e)}, \qquad Mo(G,x) = \sum_{e=uv\in E(G)} x^{|n_u(e)-n_v(e)|},$$
$$PI(G,x) = \sum_{e=uv\in E(G)} x^{m_u(e)+m_v(e)}, \quad Sz_e(G,x) = \sum_{e=uv\in E(G)} x^{m_u(e)m_v(e)}.$$

Some investigations on these polynomials can be found, for example, in [8, 22, 23, 35, 36, 38]. In addition, as for the Szeged-like indices, the weighted versions of polynomials can be also considered [9]. If $\deg(u)$ and $\deg(v)$ are the degrees of vertices u and v, then the *weighted-product Szeged polynomial* $w^*Sz(G,x)$ and the *weighted-plus Szeged polynomial* $w^+Sz(G,x)$ are defined with the following formulas:

$$\begin{aligned} w^*Sz(G,x) &= \sum_{e=uv\in E(G)} \deg(u)\deg(v) x^{n_u(e)n_v(e)}, \\ w^+Sz(G,x) &= \sum_{e=uv\in E(G)} (\deg(u)+\deg(v)) x^{n_u(e)n_v(e)}. \end{aligned}$$

It is worth mentioning that graph polynomials provide much more information about a graph than corresponding topological indices, since a polynomial is defined by several numbers (coefficients) which are themselves topological descriptors. Note also that Szeged-like polynomials were very recently used to introduce so-called root-indices of graphs, which have better discrimination power than the corresponding standard topological indices [14].

A powerful tool for efficiently calculating various distance-based topological indices is the well-known cut method [33]. In recent years, the cut method was investigated in many papers also for Szeged-like topological indices, see [3–6, 15, 34, 42] as an example. Moreover, the efficacy of the cut method was considered in [7]. On the other hand, to the best knowledge of authors of this paper, the cut method for distance-based graph polynomials has never appeared in the literature. Therefore, the aim of this paper is to fill this gap and provide the cut method for Szeged-like polynomials. For this reason, we firstly define a general concept of the Szeged-like polynomial for any connected strength-weighted graph, which includes all the above mentioned polynomials and also infinitely many other graph polynomials.

The paper reads as follows. In the next section, we present some basic concepts about relation Θ and quotient graphs. In Section 3, the strength-weighted graphs are described and the general Szeged-like polynomial is introduced. In addition, relation between Szeged-like polynomials and Szeged-like topological indices is pointed out. The main result of the paper is proved in Section 4. More precisely, we show that the Szeged-like polynomial of any connected strength-weighted graph can be computed by using the polynomials of strength-weighted quotient graphs. Finally, in the last section the developed cut method is applied to two infinite families of molecular graphs: para-polyphenyl chains and carbon nanocones.

2 Preliminaries

In this section, we define some basic concepts from graph theory. More information can be found, for example, in [27].

For a simple graph G, we denote by $V(G)$ the set of vertices and by $E(G)$ the set of edges. Moreover, we denote by $d_G(x, y)$ the usual *distance* between vertices x and y of a graph G and by $\deg(x)$ the *degree* of x. In addition, the distance between a vertex x and an edge $e = uv$ of G is defined as

$$d_G(x,e) = \min\{d_G(x,u), d_G(x,v)\}.$$

Next, we define the well-known Djoković-Winkler relation Θ on the set of edges of a connected graph, for more information see [27]. Let $e_1 = u_1v_1$ and $e_2 = u_2v_2$ be two edges of a connected graph G. Then, e_1 and e_2 are in relation Θ, denoted as $e_1\Theta e_2$, if

$$d_G(u_1,u_2) + d_G(v_1,v_2) \neq d_G(u_1,v_2) + d_G(u_2,v_1).$$

It turns out that this relation is reflexive and symmetric, but not always transitive. Therefore, by Θ^* we denote the transitive closure of relation Θ (i.e. the smallest transitive relation containing Θ). The partition $\mathcal{F} = \{F_1,\ldots,F_r\}$ of the set $E(G)$ with respect to the equivalence relation Θ^* will be referred to as Θ^*-*partition* and any set F_i is known as Θ^*-*class*. Moreover, any other partition $\mathcal{E} = \{E_1,\ldots,E_k\}$ of $E(G)$ is *coarser* than $\mathcal{F}$ if for every $i \in \{1,\ldots,k\}$ the set E_i is the union of one or more Θ^*-classes of G. In this case, we say that $\mathcal{E}$ is a *c-partition* of the set $E(G)$ [15].

Finally, we define the concept of a quotient graph [27]. Let G be a connected graph and $F \subseteq E(G)$ a subset of its edges. By $G \setminus F$ we denote the graph obtained from G by removing all the edges in F. The *quotient graph* G/F has connected components of the graph $G \setminus F$ for vertices. Moreover, two such vertices (components) X and Y are adjacent in G/F if and only if there exists $x \in V(X)$ and $y \in V(Y)$ such that x and y are adjacent in G. In addition, if $E = XY$ is an edge in G/F, we write $\widehat{E}$ to denote the set of edges of G that have one end-vertex in X and the other end-vertex in Y, i.e. $\widehat{E} = \{xy \in E(G) \,|\, x \in V(X), y \in V(Y)\}$.

3 Szeged-like topological indices and polynomials of strength-weighted graphs

In [3], authors defined the *strength-weighted graph* as a triple $G_{sw} = (G, SW_V, SW_E)$, where G is a simple graph and SW_V, SW_E are pairs of weights on vertices and edges of G, respectively:

- $SW_V = (w_v, s_v)$, where $w_v, s_v : V(G_{sw}) \to \mathbb{R}_0^+$,
- $SW_E = (w_e, s_e)$, where $w_e, s_e : E(G_{sw}) \to \mathbb{R}_0^+$.

We also recall that a strength-weighted graph G_{sw} is *normally strength-weighted* [15], if $w_v \equiv 1$, $s_e \equiv 1$, $s_v \equiv 0$, and for w_e one of the following options holds true:

(*i*) $w_e \equiv 1$,

(*ii*) $w_e(e) = \deg(u) + \deg(v)$ for any $e = uv$ (in this case, we often use $w_e^+(e)$),

(*iii*) $w_e(e) = \deg(u)\deg(v)$ for any $e = uv$ (in this case, we often use $w_e^*(e)$).

Let $e = uv \in E(G)$ be an edge of a connected graph G. The following sets are needed for the definition of the Szeged-like topological index:

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

Moreover, if G_{sw} is a connected strength-weighted graph and $e = uv$ an edge of G_{sw}, we set [15]:

$$\begin{aligned}
n_u(e|G_{sw}) &= \sum_{x \in N_u(e|G_{sw})} w_v(x),\\
m_u(e|G_{sw}) &= \sum_{x \in N_u(e|G_{sw})} s_v(x) + \sum_{f \in M_u(e|G_{sw})} s_e(f),
\end{aligned}$$

$$\begin{aligned} n_0(e|G_{sw}) &= \sum_{x \in N_0(e|G_{sw})} w_v(x), \\ m_0(e|G_{sw}) &= \sum_{x \in N_0(e|G_{sw})} s_v(x) + \sum_{f \in M_0(e|G_{sw})} s_e(f). \end{aligned}$$

The numbers $n_v(e|G_{sw})$ and $m_v(e|G_{sw})$ are defined in a similar way.

Finally, a regular function of six variables for a strength-weighted graph was introduced in [15]. Let $X \subseteq \mathbb{R}^6$ and let $F : X \to \mathbb{R}$ be a function such that $F(x_1, x_2, x_3, x_4, x_5, x_6) = F(x_2, x_1, x_4, x_3, x_5, x_6)$ for all $(x_1, x_2, x_3, x_4, x_5, x_6) \in X$. Also, for any edge $e = uv$ of a connected strength-weighted graph G_{sw} we define:

$$\begin{aligned} F(e|G_{sw}) &= F\big(n_u(e|G_{sw}), n_v(e|G_{sw}), m_u(e|G_{sw}), m_v(e|G_{sw}), \\ &\quad n_0(e|G_{sw}), m_0(e|G_{sw})\big). \end{aligned}$$

If the number $F(e|G_{sw})$ is defined for any edge $e \in E(G_{sw})$, then F is called a *regular function* for a graph G_{sw}. Consequently, a regular function F can be considered as a real-valued function defined on the edge set of G_{sw}. With this notation, the concept of a general Szeged-like topological index has been introduced in [15]. More precisely, if F is a regular function for a strength-weighted connected graph G_{sw}, then the *Szeged-like topological index* of G_{sw} is defined as

$$TI_F(G_{sw}) = \sum_{e \in E(G)} w_e(e) F(e|G_{sw}).$$

Here, we make a step further and in a similar way define also the Szeged-like polynomial of a graph.

Definition 1. *If F is a regular function for a strength-weighted connected graph G_{sw}, then the* ***Szeged-like polynomial*** *of G_{sw}, denoted by $SzP_F(G_{sw}, x)$, is defined as*

$$SzP_F(G_{sw}, x) = \sum_{e \in E(G)} w_e(e) x^{F(e|G_{sw})}.$$

It is easy to see that many well-known distance-based polynomials are just special cases of the general Szeged-like polynomial.

To explain this more precisely, let G be a connected graph and G_{sw} the normally strength-weighted quotient graph obtained from G. Then, the weights $w_e(e)$, where $e = uv \in E(G)$, regular functions F, and the corresponding Szeged-like polynomials are shown in Table 1.

Szeged-like poly.	**regular function** F	$w_e(uv)$
Szeged poly. (Sz)	x_1x_2	1
edge-Szeged poly. (Sz_e)	x_3x_4	1
revised Szeged poly. (Sz^*)	$(x_1 + x_5/2)(x_2 + x_5/2)$	1
weigh.-pr. Sz. poly. (w^*Sz)	x_1x_2	$\deg(u)\deg(v)$
weigh.-pl. Sz. poly. (w^+Sz)	x_1x_2	$\deg(u) + \deg(v)$
PI poly. (PI)	$x_3 + x_4$	1
Mostar poly. (Mo)	$\|x_1 - x_2\|$	1
Graovac-Ghor. poly. (GG)	$\sqrt{(x_1 + x_2 - 2)/(x_1x_2)}$	1
Trinajstić poly. (NT)	$(x_1 - x_2)^2$	1

Table 1. Some Szeged-like polynomials, corresponding functions F, and weights w_e.

Moreover, we can easily show the following relation between a Szeged-like topological index and the corresponding Szeged-like polynomial.

Proposition 1. *If F is a regular function for a strength-weighted connected graph G_{sw}, then*

$$TI_F(G_{sw}) = SzP'_F(G_{sw}, 1).$$

Proof. Firstly, we compute the derivative of $SzP_F(G, x)$:

$$SzP'_F(G_{sw}, x) = \sum_{e \in E(G)} w_e(e)F(e|G_{sw})x^{F(e|G_{sw})-1}.$$

By taking $x = 1$ to the above equation, we obtain

$$SzP'_F(G_{sw}, 1) = \sum_{e \in E(G)} w_e(e) F(e|G_{sw}) = TI_F(G_{sw}),$$

which completes the proof. ■

4 The generalized cut method for Szeged-like polynomials

A method for computing a Szeged-like polynomial of a connected strength-weighted graph from the corresponding weighted quotient graphs is deduced in this section. By this result, we provide the cut method for computing infinitely many polynomials of graphs. Firstly, we have to define strength-weighted quotient graphs, see [3, 5, 15].

Let G_{sw} be a connected strength-weighted graph and let $\{E_1, \ldots, E_k\}$ be a c-partition of $E(G)$. Moreover, for $i \in \{1, \ldots, k\}$ we denote by $G_{sw}/E_i = (G/E_i, SW_v^i, SW_e^i)$ the strength-weighted quotient graph, where the weights w_v^i, s_v^i, w_e^i, and s_e^i are defined as follows:

- $w_v^i : V(G_{sw}/E_i) \to \mathbb{R}_0^+$, $w_v^i(X) = \sum_{x \in V(X)} w_v(x)$, $\forall\ X \in V(G_{sw}/E_i)$,
- $s_v^i : V(G_{sw}/E_i) \to \mathbb{R}_0^+$, $s_v^i(X) = \sum_{f \in E(X)} s_e(f) + \sum_{x \in V(X)} s_v(x)$, $\forall\ X \in V(G_{sw}/E_i)$,
- $w_e^i : E(G_{sw}/E_i) \to \mathbb{R}_0^+$, $w_e^i(E) = \sum_{e \in \widehat{E}} w_e(e)$, $\forall\ E \in E(G_{sw}/E_i)$,
- $s_e^i : E(G_{sw}/E_i) \to \mathbb{R}_0^+$, $s_e^i(E) = \sum_{e \in \widehat{E}} s_e(e), \forall\ E \in E(G_{sw}/E_i)$.

It was noted in [15] that if G_{sw} is a normally strength-weighted graph, then we have:

- $w_v^i(X)$ is the number of vertices in a connected component X of $G_{sw} \setminus E_i$,

- $s_v^i(X)$ is the number of edges in a connected component X of $G_{sw} \backslash E_i$,
- $s_e^i(E) = \left|\widehat{E}\right|$ for $E \in E(G_{sw}/E_i)$. This means that if $E = XY$, then $s_e^i(E)$ is the number of edges between connected components X and Y of $G_{sw} \setminus E_i$.
- for $w_e^i(E)$, where $E \in E(G_{sw}/E_i)$, one of the following options holds true:

  (i) if $w_e \equiv 1$, then $w_e^i(E) = s_e^i(E)$,

  (ii) if $w_e = w_e^+$, then $w_e^i(E) = \sum_{e=uv \in \widehat{E}} (\deg(u) + \deg(v))$,

  (iii) if $w_e = w_e^*$, then $w_e^i(E) = \sum_{e=uv \in \widehat{E}} \deg(u) \deg(v)$.

In the rest of the paper, we will shortly write G_i to denote the quotient graph G_{sw}/E_i, where $i \in \{1, \ldots, k\}$. Also, for any vertex $u \in V(G)$ and $i \in \{1, \ldots, k\}$, let $\ell_i(u)$ be the connected component of the graph $G \setminus E_i$ that contains u.

The following two lemmas will be applied in the proof of the main theorem.

Lemma 1. *[4, 15] Let G_{sw} be a connected strength-weighted graph. Moreover, if $e = uv \in E_i$, where $i \in \{1, \ldots, k\}$, $U = \ell_i(u)$, $V = \ell_i(v)$, and $E = UV \in E(G_i)$, then*

(i) $n_u(e|G_{sw}) = n_U(E|G_i)$ *and* $n_v(e|G_{sw}) = n_V(E|G_i)$,

(ii) $m_u(e|G_{sw}) = m_U(E|G_i)$ *and* $m_v(e|G_{sw}) = m_V(E|G_i)$,

(iii) $n_0(e|G_{sw}) = n_0(E|G_i)$ *and* $m_0(e|G_{sw}) = m_0(E|G_i)$.

By Lemma 1 one can immediately obtain the following result.

Lemma 2. *[15] Let G_{sw} be a connected strength-weighted graph and F a regular function for G_{sw}. If $e = uv \in E_i$, where $i \in \{1, \ldots, k\}$, $U = \ell_i(u)$, $V = \ell_i(v)$, and $E = UV \in E(G_i)$, then*

$$F(e|G_{sw}) = F(E|G_i).$$

Finally, we can prove the main theorem which states that a Szeged-like polynomial of a strength-weighted graph can be computed as the sum of corresponding polynomials of strength-weighted quotient graphs.

Theorem 2. *Let G_{sw} be a connected strength-weighted graph. Moreover, if $\{E_1, \ldots, E_k\}$ is a c-partition of $E(G_{sw})$ and F a regular function for G_{sw}, then*

$$SzP_F(G_{sw}, x) = \sum_{i=1}^{k} SzP_F(G_i, x).$$

Proof. We follow similar reasoning as in the proof of Theorem 4.5 from [15]. It is easy to see that $E(G) = \bigcup_{i=1}^{k} E_i$. Moreover, for any $i \in \{1, \ldots, k\}$ it holds

$$E_i = \bigcup_{E \in E(G_i)} \widehat{E}.$$

By using Lemma 2 we obtain

$$\begin{aligned} SzP_F(G_{sw}, x) &= \sum_{e \in E(G_{sw})} w_e(e) x^{F(e|G_{sw})} \\ &= \sum_{i=1}^{k} \left(\sum_{e \in E_i} w_e(e) x^{F(e|G_{sw})} \right) \\ &= \sum_{i=1}^{k} \left(\sum_{E \in E(G_i)} \left[\sum_{e \in \widehat{E}} w_e(e) x^{F(e|G_{sw})} \right] \right) \\ &= \sum_{i=1}^{k} \left(\sum_{E \in E(G_i)} \left[\sum_{e \in \widehat{E}} w_e(e) x^{F(E|G_i)} \right] \right) \end{aligned}$$

$$= \sum_{i=1}^{k} \left(\sum_{E \in E(G_i)} \left[\sum_{e \in \widehat{E}} w_e(e) \right] x^{F(E|G_i)} \right)$$

$$= \sum_{i=1}^{k} \left(\sum_{E \in E(G_i)} w_e^i(E) x^{F(E|G_i)} \right)$$

$$= \sum_{i=1}^{k} SzP_F(G_i, x),$$

which is what we wanted to prove. ■

5 Applications to molecular graphs

In this final section, we present applications of the developed cut method on two families of molecular graphs. In particular, by using the weighted quotient graphs we compute the Szeged polynomial, the Mostar polynomial, the weighted-product Szeged polynomial, the weighted-plus Szeged polynomial, and the PI polynomial of para-polyphenyl chains and carbon nanocones.

5.1 Para-polyphenyl chains

Here we consider a family of chemical graphs called *para-polyphenyl chains* [41]. We denote them as PPC_n, where $n \geq 2$. Every such graph is a disjoint union of hexagons $H_1, H_2, \ldots, H_n$, where H_i and H_{i+1} are joined by an edge for any $i \in \{1, 2, \ldots, n-1\}$. More precisely, for every hexagon H_i, $i \in \{2, \ldots, n-1\}$, (which is connected to exactly two other hexagons) the two vertices of H_i of degree 3 should be at distance 3. An example of para-polyphenyl chain with 4 hexagons is depicted in Figure 1.

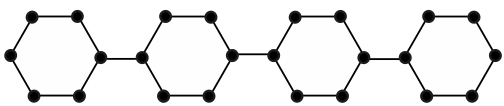

Figure 1. Para-polyphenyl chain PPC_4.

In the following, we deduce formulas for the desired polynomials of PPC_n. For this purpose, suppose that PPC_n is drawn in the plane in such a way that all the hexagons are regular and that exactly two edges on every hexagon are horizontal. The edges of hexagons of PPC_n have three different directions and the corresponding sets of these edges will be denoted by F_1, F_2, and F_3 (the set F_3 contains horizontal edges). Moreover, let F_4 be the set all the edges of PPC_n with one end-vertex in one hexagon and the other end-vertex in another hexagon. It follows by Lemma 4.3 in [41] that $\{F_1, F_2, F_3, F_4\}$ is a c-partition of the edge set of PPC_n. It is easy to see that the quotient graphs $G_i = PPC_n/F_i$, $i \in \{1, 2, 3, 4\}$, are all paths, and that G_1, G_2, G_3 are pairwise isomorphic. We will also use the same notation G_i, $i \in \{1, 2, 3, 4\}$, for corresponding strength-weighted quotient graphs.

In particular, we assume that the para-polyphenyl chains are normally strength-weighted. Since our polynomials differ in the value of the weight w_e, we consider three separate cases. For Szeged, Mostar, and PI polynomial we have $w_e(e) = 1$ for any edge e. For weighted-product Szeged polynomial we take $w_e = w_e^*$ and for the weighted-plus Szeged polynomial, this weight is defined as $w_e = w_e^+$. The corresponding strength-weighted quotient paths are depicted in Figure 2. Note, that for the sets F_1 and F_2 we obtain the same strength-weighted quotient paths.

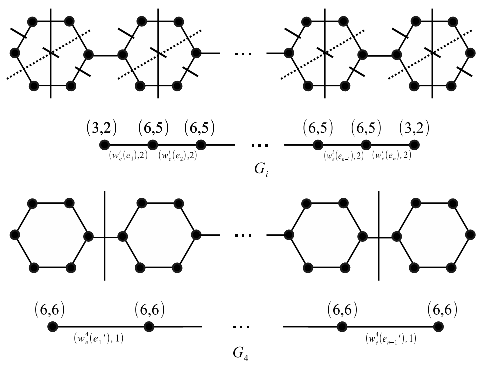

Figure 2. Strength-weighted quotient graphs G_i, $i \in \{1, 2, 3\}$, and G_4 of the graph PPC_n.

The values of weights w_v, s_v, and s_e are shown in Figure 2. Since for the selected graph polynomials different weights w_e are needed, we next consider these quantities. Let e_j, $j \in \{1, 2, \ldots, n\}$, be the edge of the quotient graph G_i, $i \in \{1, 2, 3\}$, see Figure 2. Then it holds:

- $w_e^i(e_j) = s_e^i(e_j) = 2$ for every j, where $w_e \equiv 1$ and $i \in \{1, 2, 3\}$,
- $w_e^i(e_1) = w_e^i(e_n) = 10$, where $w_e = w_e^*$ and $i \in \{1, 2\}$,
- $w_e^i(e_j) = 12$ for every $j \in \{2, \ldots, n-1\}$, where $w_e = w_e^*$ and $i \in \{1, 2\}$,
- $w_e^i(e_1) = w_e^i(e_n) = 9$, where $w_e = w_e^+$ and $i \in \{1, 2\}$,
- $w_e^i(e_j) = 10$ for every $j \in \{2, \ldots, n-1\}$, where $w_e = w_e^+$ and $i \in \{1, 2\}$,
- $w_e^3(e_j) = 8$ for every j, where $w_e = w_e^*$ or $w_e = w_e^+$.

Similarly, if e_l', $l \in \{1, \ldots, n-1\}$, is the edge of the quotient graph G_4, then we have:

- $w_e^4(e_l') = s_e^4(e_l') = 1$ for every l, where $w_e \equiv 1$,
- $w_e^4(e_l') = 9$ for every l, where $w_e = w_e^*$,
- $w_e^4(e_l') = 6$ for every l, where $w_e = w_e^+$.

By using these weights and assuming that $n \geq 2$, the corresponding polynomials of G_i, $i \in \{1, 2\}$, can be deduced:

$$Sz(G_i, x) = \begin{cases} 4 \cdot \sum_{j=1}^{\frac{n-1}{2}} x^{(6j-3)(6(n-j)+3)} + 2x^{9n^2} & ; n \text{ is odd} \\ 4 \cdot \sum_{j=1}^{\frac{n}{2}} x^{(6j-3)(6(n-j)+3)} & ; n \text{ is even,} \end{cases}$$

$$Mo(G_i, x) = \begin{cases} 4 \cdot \sum_{j=1}^{\frac{n-1}{2}} x^{6n-12j+6} + 2 & ; n \text{ is odd} \\ 4 \cdot \sum_{j=1}^{\frac{n}{2}} x^{6n-12j+6} & ; n \text{ is even,} \end{cases}$$

$$w^*Sz(G_i,x) = \begin{cases} 24\cdot\sum_{j=2}^{\frac{n-1}{2}} x^{(6j-3)(6(n-j)+3)} \\ +20x^{18n-9}+12x^{9n^2} & ; n \text{ is odd} \\ 24\cdot\sum_{j=2}^{\frac{n}{2}} x^{(6j-3)(6(n-j)+3)} \\ +20x^{18n-9} & ; n \text{ is even,} \end{cases}$$

$$w^+Sz(G_i,x) = \begin{cases} 20\cdot\sum_{j=2}^{\frac{n-1}{2}} x^{(6j-3)(6(n-j)+3)} \\ +18x^{18n-9}+10x^{9n^2} & ; n \text{ is odd} \\ 20\cdot\sum_{j=2}^{\frac{n}{2}} x^{(6j-3)(6(n-j)+3)} \\ +18x^{18n-9} & ; n \text{ is even,} \end{cases}$$

$$PI(G_i,x) = 2nx^{7n-3}.$$

Similarly, for $n \geq 2$ we get:

$$Sz(G_3,x) = \begin{cases} 4\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{(6j-3)(6(n-j)+3)} + 2x^{9n^2} & ; n \text{ is odd} \\ 4\cdot\sum_{j=1}^{\frac{n}{2}} x^{(6j-3)(6(n-j)+3)} & ; n \text{ is even,} \end{cases}$$

$$Mo(G_3,x) = \begin{cases} 4\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{6n-12j+6} + 2 & ; n \text{ is odd} \\ 4\cdot\sum_{j=1}^{\frac{n}{2}} x^{6n-12j+6} & ; n \text{ is even,} \end{cases}$$

$$w^*Sz(G_3,x) = \begin{cases} 16\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{(6j-3)(6(n-j)+3)} + 8x^{9n^2} & ; n \text{ is odd} \\ 16\cdot\sum_{j=1}^{\frac{n}{2}} x^{(6j-3)(6(n-j)+3)} & ; n \text{ is even,} \end{cases}$$

$$w^+Sz(G_3,x) = \begin{cases} 16\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{(6j-3)(6(n-j)+3)} + 8x^{9n^2} & ; n \text{ is odd} \\ 16\cdot\sum_{j=1}^{\frac{n}{2}} x^{(6j-3)(6(n-j)+3)} & ; n \text{ is even,} \end{cases}$$

$$PI(G_3,x) = 2nx^{7n-3}.$$

Moreover, for $n \geq 2$ we also obtain the polynomials of G_4:

$$Sz(G_4,x) = \begin{cases} 2\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{36j(n-j)} & ; n \text{ is odd} \\ 2\cdot\sum_{j=1}^{\frac{n-2}{2}} x^{36j(n-j)} + x^{9n^2} & ; n \text{ is even,} \end{cases}$$

$$Mo(G_4,x) = \begin{cases} 2\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{6n-12j} & ; n \text{ is odd} \\ 2\cdot\sum_{j=1}^{\frac{n-2}{2}} x^{6n-12j} + 1 & ; n \text{ is even,} \end{cases}$$

$$w^*Sz(G_4,x) = \begin{cases} 18\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{36j(n-j)} & ;n \text{ is odd} \\ 18\cdot\sum_{j=1}^{\frac{n-2}{2}} x^{36j(n-j)} + 9x^{9n^2} & ;n \text{ is even,} \end{cases}$$

$$w^+Sz(G_4,x) = \begin{cases} 12\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{36j(n-j)} & ;n \text{ is odd} \\ 12\cdot\sum_{j=1}^{\frac{n-2}{2}} x^{36j(n-j)} + 6x^{9n^2} & ;n \text{ is even,} \end{cases}$$

$$PI(G_4,x) = (n-1)x^{7n-2}.$$

Finally, we can state the results for all five polynomials of a para-polyphenyl chain PPC_n, which are obtained by applying Theorem 2. In particular, we know that if SzP denotes any polynomial from the set $\{Sz, Mo, w^*Sz, w^+Sz, PI\}$, then

$$SzP(PPC_n,x) = 2\cdot SzP(G_1,x) + SzP(G_3,x) + SzP(G_4,x).$$

Theorem 3. *Let $n \geq 3$ be an odd number and $G = PPC_n$. Then*

$$\begin{aligned}
Sz(G,x) &= 12\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{(6j-3)(6(n-j)+3)} + 2\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{36j(n-j)} + 6x^{9n^2}, \\
Mo(G,x) &= 12\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{6n-12j+6} + 2\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{6n-12j} + 6, \\
w^*Sz(G,x) &= 64\cdot\sum_{j=2}^{\frac{n-1}{2}} x^{(6j-3)(6(n-j)+3)} + 18\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{36j(n-j)} \\
&+ 32x^{9n^2} + 56x^{18n-9}, \\
w^+Sz(G,x) &= 56\cdot\sum_{j=2}^{\frac{n-1}{2}} x^{(6j-3)(6(n-j)+3)} + 12\cdot\sum_{j=1}^{\frac{n-1}{2}} x^{36j(n-j)} \\
&+ 28x^{9n^2} + 52x^{18n-9}, \\
PI(G,x) &= 6nx^{7n-3} + (n-1)x^{7n-2}.
\end{aligned}$$

Theorem 4. *Let $n \geq 2$ be an even number and $G = PPC_n$. Then*

$$
\begin{aligned}
Sz(G,x) &= 12\cdot\sum_{j=1}^{\frac{n}{2}} x^{(6j-3)(6(n-j)+3)} + 2\cdot\sum_{j=1}^{\frac{n-2}{2}} x^{36j(n-j)} + x^{9n^2},\\
Mo(G,x) &= 12\cdot\sum_{j=1}^{\frac{n}{2}} x^{6n-12j+6} + 2\cdot\sum_{j=1}^{\frac{n-2}{2}} x^{6n-12j} + 1,\\
w^{*}Sz(G,x) &= 64\cdot\sum_{j=2}^{\frac{n}{2}} x^{(6j-3)(6(n-j)+3)} + 18\cdot\sum_{j=1}^{\frac{n-2}{2}} x^{36j(n-j)}\\
&+ 9x^{9n^2} + 56x^{18n-9},\\
w^{+}Sz(G,x) &= 56\cdot\sum_{j=2}^{\frac{n}{2}} x^{(6j-3)(6(n-j)+3)} + 12\cdot\sum_{j=1}^{\frac{n-2}{2}} x^{36j(n-j)}\\
&+ 6x^{9n^2} + 52x^{18n-9},\\
PI(G,x) &= 6nx^{7n-3} + (n-1)x^{7n-2}.
\end{aligned}
$$

From Proposition 1 it follows that by evaluating the first derivative of a Szeged-like polynomial at $x = 1$, we obtain the corresponding Szeged-like topological index. Therefore, we arrive to the final result of this subsection. It turns out that in the next corollary, the stated formulas are valid also for $n = 1$.

Corollary 1. *The Szeged index, the Mostar index, the weighted-product Szeged index, the weighted-plus Szeged index, and the PI index of* $G = PPC_n$*,* $n \geq 1$*, are equal to*

$$
\begin{aligned}
Sz(G) &= Sz'(G,1) = 42n^3 + 12n,\\
Mo(G) &= Mo'(G,1) = \begin{cases} 21n^2 - 6n - 15 & ; n \text{ is odd}\\ 21n^2 - 6n & ; n \text{ is even},\end{cases}\\
w^{*}Sz(G) &= w^{*}Sz'(G,1) = 246n^3 - 102n + 72,\\
w^{+}Sz(G) &= w^{+}Sz'(G,1) = 204n^3 - 24n + 36,\\
PI(G) &= PI'(G,1) = 49n^2 - 27n + 2.
\end{aligned}
$$

Note that some of the results stated in Corollary 1 were already derived elsewhere (for example, see [16, 41]). However, in our case these formulas are obtained by using a different approach, i.e. by applying the cut method to corresponding Szeged-like polynomials.

5.2 Carbon nanocones

In this subsection, we consider a family of *carbon nanocones* with a fixed pentagonal face as its core. More precisely, the family of carbon nanocones $CNC_5(n)$ is formed of one pentagon which is surrounded by $n \geq 1$ layers of hexagons. A representative of the mentioned family, namely $CNC_5(2)$, is depicted in Figure 3.

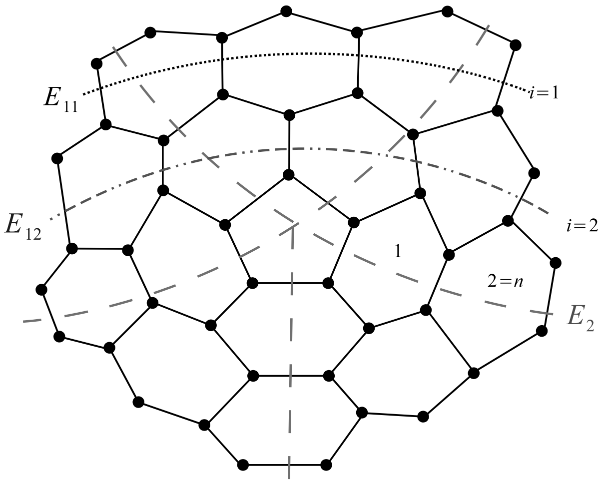

Figure 3. Carbon nanocone $CNC_5(2)$.

Our goal is to deduce formulas for the Szeged polynomial, the Mostar polynomial, the weighted-product Szeged polynomial, the weighted-plus Szeged polynomial, and PI polynomial for this infinite family of molecular graphs.

It is easy to compute that $|V(CNC_5(n))| = 5(n+1)^2$ and $|E(CNC_5(n))| = \frac{5}{2}(n+1)(3n+2)$. In [4], Mostar, edge-Mostar, and total-Mostar indices for these compounds were computed. We use some of the results stated there to calculate the above mentioned polynomials. The Θ^*-classes of $CNC_5(n)$ can therefore be seen in [4]. We denote them by E_{ji}, where $j \in \{1, \ldots, 5\}$, $i \in \{1, \ldots, n\}$, and E_2. Due to the better readability, the main representatives of Θ^*-classes of $CNC_5(2)$ are visualized in Figure 3.

In the following discussion, we suppose that $CNC_5(n)$ is the normally strength-weighted graph. Similarly as in the previous subsection, for the Szeged polynomial, the Mostar, and the PI polynomial we have $w_e \equiv 1$. On the other hand, for the weighted-product Szeged polynomial we take $w_e = w_e^*$ and for the weighted-plus Szeged polynomial we set $w_e = w_e^+$. The corresponding strength-weighted quotient graphs G_{ji} and G_2 are illustrated in Figure 4. The associated weights are written in the following propositions.

Proposition 5. *[4] For $G = CNC_5(n)$ let G_{ji} be the corresponding strength-weighted quotient graph and let $X, Y \in V(G_{ji})$, $E \in E(G_{ji})$, see Figure 4. The weights $w_v^{ji}(X)$, $s_v^{ji}(X)$, $w_v^{ji}(Y)$, $s_v^{ji}(Y)$, and $s_e^{ji}(E)$ have values*

$$\begin{aligned}
&w_v^{ji}(X) = i(i + 2n + 2), \qquad s_v^{ji}(X) = \frac{1}{2}\left(3i - 2n + 6in + 3i^2 - 2\right), \\
&w_v^{ji}(Y) = |V(G)| - w_v^{ji}(X), \quad s_v^{ji}(Y) = |E(G)| - s_v^{ji}(X) - (n + 1 + i), \\
&s_e^{ji}(E) = n + 1 + i.
\end{aligned}$$

We observe that all vertices (or edges) in the strength-weighted quotient graph G_2 have the same pair of weights. To compute the desired polynomials, the next result is also needed.

Proposition 6. *For $G = CNC_5(n)$ let G_2 be the corresponding strength-weighted quotient graph and let $X \in V(G_2)$, $E \in E(G_2)$, see Figure 4. The weights $w_v^2(X), s_e^2(E)$, and $s_v^2(X)$ have values*

$$\begin{aligned}
&w_v^2(X) = (n + 1)^2, \quad s_e^2(E) = n + 1, \\
&s_v^2(X) = \frac{1}{5}\left(|E(G)| - 5(n + 1)\right) = \frac{3n(n + 1)}{2}.
\end{aligned}$$

Again, graph polynomials differ in the weight w_e, therefore the next result is given.

Proposition 7. *If $G = CNC_5(n)$ and E is an edge of a strength-weighted quotient graph G_{ji} or G_2, then*

- $w_e^{ji}(E) = s_e^{ji}(E) = n + 1 + i$, *where* $w_e \equiv 1$,
- $w_e^{ji}(E) = 3(3n + 3i + 1)$, *where* $w_e = w_e^*$,
- $w_e^{ji}(E) = 2(3n + 3i + 2)$, *where* $w_e = w_e^+$,
- $w_e^2(E) = s_e^2(E) = n + 1$, *where* $w_e \equiv 1$,
- $w_e^2(E) = 9n + 4$, *where* $w_e = w_e^*$,
- $w_e^2(E) = 2(3n + 2)$, *where* $w_e = w_e^+$.

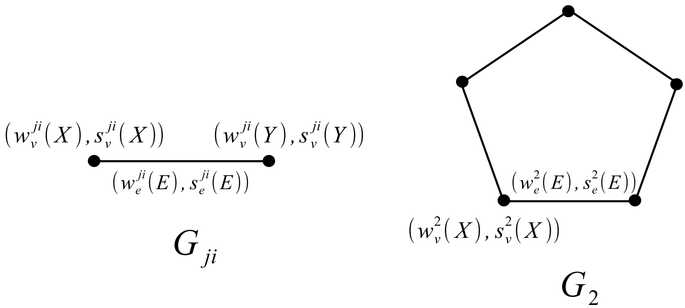

Figure 4. Quotient graphs G_{ji} and G_2 for carbon nanocone $CNC_5(n)$.

Due to Propositions 5 and 7, the corresponding polynomials of G_{ji} can be obtained:

$$\begin{aligned} Sz(G_{ji}, x) &= (n + 1 + i)x^{w_v^{ji}(X) \cdot w_v^{ji}(Y)} \\ &= (n + 1 + i)x^{i(i+2n+2)(5(n+1)^2 - i(i+2n+2))}, \\ Mo(G_{ji}, x) &= (n + 1 + i)x^{|w_v^{ji}(X) - w_v^{ji}(Y)|} \\ &= (n + 1 + i)x^{|i(i+2n+2) - (5(n+1)^2 - i(i+2n+2))|} \\ &= (n + 1 + i)x^{5(1+n)^2 - 2i(2+i+2n)}, \end{aligned}$$

$$
\begin{aligned}
w^*Sz(G_{ji},x) &= 3(3n+3i+1)x^{w_v^{ji}(X)\cdot w_v^{ji}(Y)} \\
&= 3(3n+3i+1)x^{i(i+2n+2)(5(n+1)^2-i(i+2n+2))}, \\
w^+Sz(G_{ji},x) &= 2(3n+3i+2)x^{w_v^{ji}(X)\cdot w_v^{ji}(Y)} \\
&= 2(3n+3i+2)x^{i(i+2n+2)(5(n+1)^2-i(i+2n+2))}, \\
PI(G_{ji},x) &= (n+1+i)x^{s_v^{ji}(X)+s_v^{ji}(Y)} \\
&= (n+1+i)x^{s_v^{ji}+|E(G)|-s_v^{ji}(X)-(n+1+i)} \\
&= (n+1+i)x^{\frac{5}{2}(n+1)(3n+2)-(n+1+i)}.
\end{aligned}
$$

Similarly, by Propositions 6 and 7, the corresponding polynomials of G_2 are:

$$
\begin{aligned}
Sz(G_2,x) &= 5\cdot(n+1)x^{2(n+1)^2\cdot 2(n+1)^2} = 5(n+1)x^{4(n+1)^4}, \\
Mo(G_2,x) &= 0 \\
w^*Sz(G_2,x) &= 5\cdot(9n+4)x^{2(n+1)^2\cdot 2(n+1)^2} = 5(9n+4)x^{4(n+1)^4}, \\
w^+Sz(G_2,x) &= 5\cdot 2(3n+2)x^{2(n+1)^2\cdot 2(n+1)^2} = 10(3n+2)x^{4(n+1)^4}, \\
PI(G_2,x) &= 5\cdot(n+1)x^{4\cdot\frac{3n(n+1)}{2}+4(n+1)} = 5(n+1)x^{6n^2+10n+4}.
\end{aligned}
$$

Finally, by using the main result, Theorem 2, we obtain the following theorem.

Theorem 8. *For carbon nanocone $G = CNC_5(n)$, where $n \geq 1$, it holds*

$$
\begin{aligned}
Sz(G,x) &= 5\cdot\sum_{i=1}^{n} Sz(G_{ji},x) + Sz(G_2,x) \\
&= 5\cdot\sum_{i=1}^{n}(n+1+i)x^{i(i+2n+2)(5(n+1)^2-i(i+2n+2))} \\
&+ 5(n+1)x^{4(n+1)^4},
\end{aligned}
$$

$$\begin{aligned}
Mo(G,x) &= 5\cdot\sum_{i=1}^{n} Mo(G_{ji},x) + Mo(G_2,x)\\
&= 5\cdot\sum_{i=1}^{n}(n+1+i)x^{5(n+1)^2-2i(2+i+2n)},\\
w^{*}Sz(G,x) &= 5\cdot\sum_{i=1}^{n} w^{*}Sz(G_{ji},x) + w^{*}Sz(G_2,x)\\
&= 5\cdot\sum_{i=1}^{n} 3(3n+3i+1)x^{i(i+2n+2)(5(n+1)^2-i(i+2n+2))}\\
&+ 5(9n+4)\cdot x^{4(n+1)^4},\\
w^{+}Sz(G,x) &= 5\cdot\sum_{i=1}^{n} w^{+}Sz(G_{ji},x) + w^{+}Sz(G_2,x)\\
&= 5\cdot\sum_{i=1}^{n} 2(3n+3i+2)x^{i(i+2n+2)(5(n+1)^2-i(i+2n+2))}\\
&+ 10(3n+2)\cdot x^{4(n+1)^4},\\
PI(G,x) &= 5\cdot\sum_{i=1}^{n} PI(G_{ji},x) + PI(G_2,x)\\
&= 5\cdot\sum_{i=1}^{n}(n+1+i)x^{\frac{5}{2}(n+1)(3n+2)-(n+1+i)}\\
&+ 5(n+1)x^{6n^2+10n+4}.
\end{aligned}$$

Like in the subsection before we compute the first derivative of a Szeged-like polynomial at $x = 1$, which gives the corresponding Szeged-like topological index. Therefore, the last result can be used to obtain the next corollary (again, some of these results were already obtained elsewhere, see [4, 12]).

Corollary 2. *The Szeged index, the Mostar index, the weighted-product Szeged index, the weighted-plus Szeged index, and the PI index of* $G = CNC_5(n)$ *are equal to*

$$
\begin{aligned}
Sz(G) &= Sz'(CNC_5(n),1)\\
&= \frac{1}{4}\big(135n^6+770n^5+1805n^4+2220n^3\\
&+ 1510n^2+540n+80\big),\\
Mo(G) &= Mo'(CNC_5(n),1)\\
&= \frac{n}{2}\big(30n^3+105n^2+120n+45\big),\\
w^*Sz(G) &= w^*Sz'(CNC_5(n),1)\\
&= \frac{1}{4}\big(1215n^6+6434n^5+13725n^4+15000n^3\\
&+ 8810n^2+2636n+320\big),\\
w^+Sz(G) &= w^+Sz'(CNC_5(n),1)\\
&= \frac{1}{6}\big(1215n^6+6682n^5+14945n^4+17330n^3\\
&+ 10960n^2+3588n+480\big),\\
PI(G) &= PI'(CNC_5(n),1) =\\
&= \frac{1}{12}\big(675n^4+2020n^3+2265n^2+1160n+240\big).
\end{aligned}
$$

6 Conclusion

In the present paper we introduced a concept of the general Szeged-like polynomial which includes, for example, the Szeged polynomial, weighted Szeged polynomials, the edge-Szeged polynomial, the PI polynomial, the Mostar polynomial, etc. This general polynomial was defined for a connected strength-weighted graph, which includes two weights on the vertices and two weights on the edges of a given graph. We were able to deduce a method for calculating any such polynomial by computing the same polynomials on strength-weighted quotient graphs, which represents a new approach to the investigation of distance-based graph polynomials. Since our method is very general, we presented how it can be used to compute various Szeged-like polynomials or topological indices on some important families of chemical graphs.

It is also worth mentioning that by using the developed method, one can calculate various Szeged-like polynomials of benzenoid systems, phenylenes and tree-like polyphenyls in linear time $O(n)$ with respect to the number of vertices n of a given graph (if we work in the model where addition of polynomials can be performed in constant time). To prove such results, one can use similar reasoning as for some topological indices (for example, see [15, 18, 41, 42]) and the details are therefore omitted.

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