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COMPUTING SOME TOPOLOGICAL INDICES OF ROOTED PRODUCT OF GRAPHS

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In this paper, exact formulas for computing the Szeged index, vertex PI index, weighted Szeged index, weighted vertex PI index, and revised Szeged index of rooted product of two graphs are presented. Results are applied to compute these indices for some chemical graphs by specializing components in rooted products.

Keywords: Szeged index, vertex PI index, weighted Szeged index, weighted vertex PI index, revised Szeged index, rooted product of graphs

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. We denote by $d(u|G)$ the degree of the vertex u in G and by $d(u,v|G)$ the distance between the vertices u and v in G. Let $e=uv$ be the edge of G connecting the vertices u and v. The quantities $n_0(e|G)$, $n_u(e|G)$, and $n_v(e|G)$ are defined to be the number of vertices of G equidistant from u and v, the number of vertices of G lying closer to u than to v, and the number of vertices of G lying closer to v than to u, respectively, i.e.,

$$n_0(e|G) = \left|\{z \in V(G) : d(z,u|G) = d(z,v|G)\}\right|,$$

$$n_u(e|G) = \left|\{z \in V(G) : d(z,u|G) < d(z,v|G)\}\right|,$$

$$n_v(e|G) = \left|\{z \in V(G) : d(z,v|G) < d(z,u|G)\}\right|.$$

For the vertex $z \in V(G)$, we define

$$m_z(G) = \left|\{e = uv \in E(G) : d(u,z|G) \neq d(v,z|G)\}\right|.$$

Chemical graphs are models of molecules in which atoms are represented by vertices and chemical bonds by edges of a graph. A *topological index* is any function on a chemical graph irrespective of the labeling of its vertices. The best known and widely used topological index is the *Wiener index*. This index was introduced in 1947 by Wiener [16] who used it for modeling the thermodynamic properties of alkanes. The Wiener index of a chemical graph represents the sum of distances between all pairs of its atoms/vertices.

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Motivated by the original definition of the Wiener index of a tree, Gutman [9] introduced the *Szeged index*, which coincides with the Wiener index for a tree. It found applications in quantitative structure-property-activity-toxicity modeling [13]. The Szeged index of a graph G is defined as

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

In recent years, some variants of the Szeged index such as the *vertex PI index* [14], *weighted Szeged index* [10], *weighted vertex PI index* [10], and *revised Szeged index* [15] have been introduced and studied by both mathematicians and chemists. These indices are defined for a graph G as follows.

$$PI_v(G) = \sum_{e=uv\in E(G)} [n_u(e|G) + n_v(e|G)],$$

$$Sz_w(G) = \sum_{e=uv\in E(G)} [d(u|G) + d(v|G)]n_u(e|G)n_v(e|G),$$

$$PI_w(G) = \sum_{e=uv\in E(G)} [d(u|G) + d(v|G)][n_u(e|G) + n_v(e|G)],$$

$$Sz^*(G) = \sum_{e=uv\in E(G)} [n_u(e|G) + \frac{n_0(e|G)}{2}][n_v(e|G) + \frac{n_0(e|G)}{2}].$$

We refer the reader to [1,7,8,12] for more information on these indices.

The *rooted product* $G_1\{G_2\}$ of a graph G_1 and a rooted graph G_2 is the graph obtained by taking one copy of G_1 and $|V(G_1)|$ copies of G_2, and by identifying the root vertex of the *i*-th copy of G_2 with the *i*-th vertex of G_1, for $i = 1,2,...,|V(G_1)|$.

In this paper, the Szeged index, vertex PI index, weighted Szeged index, weighted vertex PI index, and revised Szeged index of rooted product of graphs are computed. For more information on computing topological indices of rooted product see [2-6,11,17].

2. Results and discussion

Let G_1 and G_2 be two simple connected graphs with vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$, respectively. In this section, we compute the Szeged index, vertex PI index, weighted Szeged index, weighted vertex PI index, and revised Szeged index of the rooted product of G_1 and G_2. Throughout this section, we denote the root vertex of G_2 by x and the degree of x in G_2 by δ. Also, we denote by n_i and m_i, the order and size of the graph G_i, respectively, where $i \in \{1,2\}$. In addition, for notational convenience, we define

$$\overline{N} = \sum_{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)} n_v(e|G_2)\ ,\ \underline{N} = \sum_{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)} n_u(e|G_2)\ ,$$

$$N(x) = \sum_{e=xv\in E(G_2)} n_v(e|G_2),\ Sz(x) = \sum_{e=xv\in E(G_2)} n_x(e|G_2)n_v(e|G_2),$$

$$PI_v(x) = \sum_{e=xv\in E(G_2)} [n_x(e|G_2) + n_v(e|G_2)].$$

Theorem 2.1 The Szeged index of the rooted product $G_1\{G_2\}$ is given by

$$Sz(G_1\{G_2\}) = {n_2}^2 Sz(G_1) + n_1 Sz(G_2) + n_1 n_2 (n_1 - 1)\overline{N}\ . \qquad (1)$$

Proof. From the definition of the Szeged index, we have

$$Sz(G_1\{G_2\}) = \sum_{e=uv\in E(G_1\{G_2\})} n_u(e|G_1\{G_2\})n_v(e|G_1\{G_2\}).$$

We partition the above sum into two sums as follows.

The first sum S_1 consists of contributions to $Sz(G_1\{G_2\})$ of edges from G_1,

$$S_1 = \sum_{e=uv\in E(G_1)} n_u(e|G_1\{G_2\})n_v(e|G_1\{G_2\}).$$

By definition of rooted product, we have

$$S_1 = \sum_{e=uv\in E(G_1)} [n_2 n_u(e|G_1)][n_2 n_v(e|G_1)] = {n_2}^2 \sum_{e=uv\in E(G_1)} n_u(e|G_1)n_v(e|G_1) = {n_2}^2 Sz(G_1).$$

The second sum S_2 consists of contributions to $Sz(G_1\{G_2\})$ of edges from n_1 copies of G_2,

$$S_2 = n_1 \sum_{e=uv\in E(G_2)} n_u(e|G_1\{G_2\})n_v(e|G_1\{G_2\}).$$

By definition of rooted product, we have

$$S_2 = n_1 \sum_{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)} [n_u(e|G_2) + n_2(n_1-1)]n_v(e|G_2)$$
$$+ n_1 \sum_{e=uv\in E(G_2):d(u,x|G_2)=d(v,x|G_2)} n_u(e|G_2)n_v(e|G_2)$$
$$= n_1\left[\sum_{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)} n_u(e|G_2)n_v(e|G_2) + \sum_{e=uv\in E(G_2):d(u,x|G_2)=d(v,x|G_2)} n_u(e|G_2)n_v(e|G_2)\right]$$
$$+ n_1 n_2(n_1-1) \sum_{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)} n_v(e|G_2) = n_1 Sz(G_2) + n_1 n_2 (n_1-1)\overline{N}\ .$$

Eq. (1) is obtained by adding the quantities S_1 and S_2. ■

Theorem 2.2 The vertex PI index of the rooted product $G_1\{G_2\}$ is given by

$$PI_v(G_1\{G_2\}) = n_2 PI_v(G_1) + n_1 PI_v(G_2) + n_1 n_2 (n_1 - 1)m_x(G_2)\ . \qquad (2)$$

Proof. From the definition of the vertex PI index, we have

$$PI_v(G_1\{G_2\}) = \sum_{e=uv\in E(G_1\{G_2\})}[n_u(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})].$$

We partition the above sum into two sums as follows.

The first sum S_1 consists of contributions to $PI_v(G_1\{G_2\})$ of edges from G_1,

$$S_1 = \sum_{e=uv\in E(G_1)}[n_u(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})].$$

By definition of rooted product, we have

$$S_1 = \sum_{e=uv\in E(G_1)}[n_2 n_u(e|G_1) + n_2 n_v(e|G_1)] = n_2 \sum_{e=uv\in E(G_1)}[n_u(e|G_1) + n_v(e|G_1)] = n_2 PI_v(G_1).$$

The second sum S_2 consists of contributions to $PI_v(G_1\{G_2\})$ of edges from n_1 copies of G_2,

$$S_2 = n_1 \sum_{e=uv\in E(G_2)}[n_u(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})].$$

By definition of rooted product, we have

$$\begin{aligned} S_2 &= n_1 \sum_{e=uv\in E(G_2):d(u,x|G_2)\neq d(v,x|G_2)}[n_u(e|G_2) + n_v(e|G_2) + n_2(n_1-1)] \\ &\quad + n_1 \sum_{e=uv\in E(G_2):d(u,x|G_2)=d(v,x|G_2)}[n_u(e|G_2) + n_v(e|G_2)] \\ &= n_1\left[\sum_{e=uv\in E(G_2):d(u,x|G_2)\neq d(v,x|G_2)}[n_u(e|G_2) + n_v(e|G_2)] + \sum_{e=uv\in E(G_2):d(u,x|G_2)=d(v,x|G_2)}[n_u(e|G_2) + n_v(e|G_2)]\right] \\ &\quad + n_1 n_2(n_1-1)\left|\{e=uv\in E(G_2): d(u,x|G_2)\neq d(v,x|G_2)\}\right| \\ &= n_1 PI_v(G_2) + n_1 n_2(n_1-1)m_x(G_2). \end{aligned}$$

Eq. (2) is obtained by adding the quantities S_1 and S_2. ■

Theorem 2.3 The weighted Szeged index of the rooted product $G_1\{G_2\}$ is given by

$$\begin{aligned} Sz_w(G_1\{G_2\}) &= n_2{}^2 Sz_w(G_1) + 2\delta n_2{}^2 Sz(G_1) + n_1 Sz_w(G_2) + 2m_1 Sz(x) \qquad (3) \\ &\quad + 2m_1 n_2(n_1-1)N(x) + n_1 n_2(n_1-1)\sum_{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)}[d(u|G_2) + d(v|G_2)]n_v(e|G_2). \end{aligned}$$

Proof. From the definition of the weighted Szeged index, we have

$$Sz_w(G_1\{G_2\}) = \sum_{e=uv\in E(G_1\{G_2\})}[d(u|G_1\{G_2\}) + d(v|G_1\{G_2\})]n_u(e|G_1\{G_2\})n_v(e|G_1\{G_2\}).$$

We partition the above sum into two sums as follows.

The first sum S_1 consists of contributions to $Sz_w(G_1\{G_2\})$ of edges from G_1,

$$S_1 = \sum_{e=uv\in E(G_1)}[d(u|G_1\{G_2\}) + d(v|G_1\{G_2\})]n_u(e|G_1\{G_2\})n_v(e|G_1\{G_2\}).$$

By definition of rooted product, we have

$$S_1 = \sum_{e=uv\in E(G_1)} [d(u|G_1)+\delta+d(v|G_1)+\delta][n_2 n_u(e|G_1)][n_2 n_v(e|G_1)]$$
$$= n_2^2 \sum_{e=uv\in E(G_1)} [d(u|G_1)+d(v|G_1)]n_u(e|G_1)n_v(e|G_1) + 2\delta n_2^2 \sum_{e=uv\in E(G_1)} n_u(e|G_1)n_v(e|G_1)$$
$$= n_2^2 Sz_w(G_1) + 2\delta n_2^2 Sz(G_1).$$

The second sum S_2 consists of contributions to $Sz_w(G_1\{G_2\})$ of edges from n_1 copies of G_2,

$$S_2 = \sum_{z\in V(G_1)} \sum_{e=uv\in E(G_2)} [d(u|G_1\{G_2\})+d(v|G_1\{G_2\})]n_u(e|G_1\{G_2\})n_v(e|G_1\{G_2\}).$$

To compute the sum S_2, we partition it into two sums S_{21} and S_{22} as follows.

The sum S_{21} is equal to

$$S_{21} = \sum_{z\in V(G_1)} \sum_{e=xv\in E(G_2)} [d(x|G_1\{G_2\})+d(v|G_1\{G_2\})]n_x(e|G_1\{G_2\})n_v(e|G_1\{G_2\}).$$

By definition of rooted product, we have

$$S_{21} = \sum_{z\in V(G_1)} \sum_{e=xv\in E(G_2)} [d(z|G_1)+\delta+d(v|G_2)][n_x(e|G_2)+n_2(n_1-1)]n_v(e|G_2)$$
$$= \sum_{z\in V(G_1)} d(z|G_1) \sum_{e=xv\in E(G_2)} n_x(e|G_2)n_v(e|G_2) + n_2(n_1-1) \sum_{z\in V(G_1)} d(z|G_1) \sum_{e=xv\in E(G_2)} n_v(e|G_2)$$
$$+ n_1 \sum_{e=xv\in E(G_2)} [\delta+d(v|G_2)]n_x(e|G_2)n_v(e|G_2)$$
$$+ n_1 n_2(n_1-1) \sum_{e=xv\in E(G_2)} [\delta+d(v|G_2)]n_v(e|G_2)$$
$$= 2m_1 Sz(x) + 2m_1 n_2(n_1-1)N(x) + n_1 \sum_{e=xv\in E(G_2)} [\delta+d(v|G_2)]n_x(e|G_2)n_v(e|G_2)$$
$$+ n_1 n_2(n_1-1) \sum_{e=xv\in E(G_2)} [\delta+d(v|G_2)]n_v(e|G_2).$$

The sum S_{22} is equal to

$$S_{22} = \sum_{z\in V(G_1)} \sum_{e=uv\in E(G_2):u,v\neq x} [d(u|G_1\{G_2\})+d(v|G_1\{G_2\})]n_u(e|G_1\{G_2\})n_v(e|G_1\{G_2\}).$$

By definition of rooted product, we have

$$S_{22} = n_1 \sum_{e=uv\in E(G_2):u,v\neq x, d(u,x|G_2)<d(v,x|G_2)} [d(u|G_2)+d(v|G_2)][n_u(e|G_2)+n_2(n_1-1)]n_v(e|G_2)$$
$$+ n_1 \sum_{e=uv\in E(G_2):d(u,x|G_2)=d(v,x|G_2)} [d(u|G_2)+d(v|G_2)]n_u(e|G_2)n_v(e|G_2)$$
$$= n_1 \Bigg[\sum_{e=uv\in E(G_2):u,v\neq x, d(u,x|G_2)<d(v,x|G_2)} [d(u|G_2)+d(v|G_2)]n_u(e|G_2)n_v(e|G_2)$$

$$+ \sum_{e=uv\in E(G_2):d(u,x|G_2)=d(v,x|G_2)} [d(u|G_2)+d(v|G_2)]n_u(e|G_2)n_v(e|G_2) \Bigg]$$

$$+ n_1 n_2 (n_1 - 1) \sum_{e=uv\in E(G_2):u,v\neq x, d(u,x|G_2)<d(v,x|G_2)} [d(u|G_2)+d(v|G_2)]n_v(e|G_2) .$$

By adding S_{21} and S_{22}, we get

$$S_2 = n_1 Sz_w(G_2) + 2m_1 Sz(x) + 2m_1 n_2 (n_1 - 1) N(x)$$
$$+ n_1 n_2 (n_1 - 1) \sum_{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)} [d(u|G_2)+d(v|G_2)]n_v(e|G_2) .$$

Eq. (3) is obtained by adding the quantities S_1 and S_2. ■

Theorem 2.4 The weighted vertex PI index of the rooted product $G_1\{G_2\}$ is given by

$$PI_w(G_1\{G_2\}) = n_2 PI_w(G_1) + 2\delta n_2 PI_v(G_1) + n_1 PI_w(G_2) + 2\delta m_1 n_2 (n_1 - 1) \quad (4)$$
$$+ 2m_1 PI_v(x) + n_1 n_2 (n_1 - 1) \sum_{e=uv\in E(G_2):d(u,x|G_2)\neq d(v,x|G_2)} [d(u|G_2)+d(v|G_2)] .$$

Proof. From the definition of the weighted vertex PI index, we have

$$PI_w(G_1\{G_2\}) = \sum_{e=uv\in E(G_1\{G_2\})} [d(u|G_1\{G_2\}) + d(v|G_1\{G_2\})][n_u(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})] .$$

We partition the above sum into two sums as follows.

The first sum S_1 consists of contributions to $PI_w(G_1\{G_2\})$ of edges from G_1,

$$S_1 = \sum_{e=uv\in E(G_1)} [d(u|G_1\{G_2\}) + d(v|G_1\{G_2\})][n_u(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})] .$$

By definition of rooted product, we have

$$S_1 = \sum_{e=uv\in E(G_1)} [d(u|G_1) + \delta + d(v|G_1) + \delta][n_2 n_u(e|G_1) + n_2 n_v(e|G_1)]$$
$$= n_2 \sum_{e=uv\in E(G_1)} [d(u|G_1) + d(v|G_1)][n_u(e|G_1) + n_v(e|G_1)]$$
$$+ 2\delta n_2 \sum_{e=uv\in E(G_1)} [n_u(e|G_1) + n_v(e|G_1)] = n_2 PI_w(G_1) + 2\delta n_2 PI_v(G_1) .$$

The second sum S_2 consists of contributions to $PI_w(G_1\{G_2\})$ of edges from n_1 copies of G_2,

$$S_2 = \sum_{z\in V(G_1)} \sum_{e=uv\in E(G_2)} [d(u|G_1\{G_2\}) + d(v|G_1\{G_2\})][n_u(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})] .$$

To compute the sum S_2, we partition it into two sums S_{21} and S_{22} as follows.

The sum S_{21} is equal to

$$S_{21} = \sum_{z\in V(G_1)} \sum_{e=xv\in E(G_2)} [d(x|G_1\{G_2\}) + d(v|G_1\{G_2\})][n_x(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})] .$$

By definition of rooted product, we have

$$S_{21} = \sum_{z\in V(G_1)} \sum_{e=xv\in E(G_2)} [d(z|G_1) + \delta + d(v|G_2)][n_2(n_1-1) + n_x(e|G_2) + n_v(e|G_2)]$$

$$= n_2(n_1-1) \sum_{z\in V(G_1)} \sum_{e=xv\in E(G_2)} [d(z|G_1) + \delta + d(v|G_2)]$$

$$+ \sum_{z\in V(G_1)} d(z|G_1) \sum_{e=xv\in E(G_2)} [n_x(e|G_2) + n_v(e|G_2)]$$

$$+ n_1 \sum_{e=xv\in E(G_2)} [\delta + d(v|G_2)][n_x(e|G_2) + n_v(e|G_2)]$$

$$= 2\delta m_1 n_2(n_1-1) + n_1 n_2(n_1-1) \sum_{e=xv\in E(G_2)} [\delta + d(v|G_2)] + 2m_1 PI_v(x)$$

$$+ n_1 \sum_{e=xv\in E(G_2)} [\delta + d(v|G_2)][n_x(e|G_2) + n_v(e|G_2)].$$

The sum S_{22} is equal to

$$S_{22} = \sum_{z\in V(G_1)} \sum_{e=uv\in E(G_2):u,v\neq x} [d(u|G_1\{G_2\}) + d(v|G_1\{G_2\})][n_u(e|G_1\{G_2\}) + n_v(e|G_1\{G_2\})].$$

By definition of rooted product, we have

$$S_{22} = n_1 \sum_{e=uv\in E(G_2):u,v\neq x, d(u,x|G_2)\neq d(v,x|G_2)} [d(u|G_2) + d(v|G_2)][n_u(e|G_2) + n_v(e|G_2) + n_2(n_1-1)]$$

$$+ n_1 \sum_{e=uv\in E(G_2):d(u,x|G_2)=d(v,x|G_2)} [d(u|G_2) + d(v|G_2)][n_u(e|G_2) + n_v(e|G_2)]$$

$$= n_1 \Bigg[\sum_{e=uv\in E(G_2):u,v\neq x, d(u,x|G_2)\neq d(v,x|G_2)} [d(u|G_2) + d(v|G_2)][n_u(e|G_2) + n_v(e|G_2)]$$

$$+ \sum_{e=uv\in E(G_2):d(u,x|G_2)=d(v,x|G_2)} [d(u|G_2) + d(v|G_2)][n_u(e|G_2) + n_v(e|G_2)] \Bigg]$$

$$+ n_1 n_2(n_1-1) \sum_{e=uv\in E(G_2):u,v\neq x, d(u,x|G_2)\neq d(v,x|G_2)} [d(u|G_2) + d(v|G_2)].$$

By adding S_{21} and S_{22}, we get

$$S_2 = n_1 PI_w(G_2) + 2\delta m_1 n_2(n_1-1) + 2m_1 PI_v(x)$$
$$+ n_1 n_2(n_1-1) \sum_{e=uv\in E(G_2):d(u,x|G_2)\neq d(v,x|G_2)} [d(u|G_2) + d(v|G_2)].$$

Eq. (4) is obtained by adding the quantities S_1 and S_2. ■

We define the *second vertex PI index* of a graph G as

$$PI_v^{(2)}(G) = \sum_{e=uv\in E(G)} [n_u(e|G)^2 + n_v(e|G)^2].$$

Theorem 2.5 [7] Let G be a graph of order *n* and size *m*. Then

$$Sz^{*}(G)=\frac{mn^{2}}{4}-\frac{1}{4}PI_{v}^{(2)}(G)+\frac{1}{2}Sz(G)\,. \qquad (5)$$

Lemma 2.6 The second vertex PI index of the rooted product $G_1\{G_2\}$ is given by

$$PI_{v}^{(2)}(G_1\{G_2\})={n_2}^{2}PI_{v}^{(2)}(G_1)+n_1PI_{v}^{(2)}(G_2)+n_1{n_2}^{2}(n_1-1)^{2}m_x(G_2) \qquad (6)$$
$$+2n_1n_2(n_1-1)\underline{N}\,.$$

Proof. From the definition of the second vertex PI index, we have

$$PI_{v}^{(2)}(G_1\{G_2\})=\sum_{e=uv\in E(G_1\{G_2\})}[n_u(e|G_1\{G_2\})^{2}+n_v(e|G_1\{G_2\})^{2}]\,.$$

We partition the above sum into two sums as follows.

The first sum S_1 consists of contributions to $PI_{v}^{(2)}(G_1\{G_2\})$ of edges in G_1,

$$S_1=\sum_{e=uv\in E(G_1)}[n_u(e|G_1\{G_2\})^{2}+n_v(e|G_1\{G_2\})^{2}]\,.$$

By definition of rooted product, we have

$$S_1=\sum_{e=uv\in E(G_1)}[(n_2n_u(e|G_1))^{2}+(n_2n_v(e|G_1))^{2}]={n_2}^{2}PI_{v}^{(2)}(G_1)\,.$$

The second sum S_2 consists of contributions to $PI_{v}^{(2)}(G_1\{G_2\})$ of edges from n_1 copies of G_2,

$$S_2=n_1\sum_{e=uv\in E(G_2)}[n_u(e|G_1\{G_2\})^{2}+n_v(e|G_1\{G_2\})^{2}]\,.$$

By definition of rooted product, we have

$$S_2=n_1\sum_{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)}[(n_u(e|G_2)+n_2(n_1-1))^{2}+n_v(e|G_2)^{2}]$$
$$+n_1\sum_{e=uv\in E(G_2):d(u,x|G_2)=d(v,x|G_2)}[n_u(e|G_2)^{2}+n_v(e|G_2)^{2}]$$
$$=n_1\left[\sum_{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)}[n_u(e|G_2)^{2}+n_v(e|G_2)^{2}]\right.$$
$$\left.+\sum_{e=uv\in E(G_2):d(u,x|G_2)=d(v,x|G_2)}[n_u(e|G_2)^{2}+n_v(e|G_2)^{2}]\right]$$
$$+n_1{n_2}^{2}(n_1-1)^{2}\left|\{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)\}\right|$$
$$+2n_1n_2(n_1-1)\sum_{e=uv\in E(G_2):d(u,x|G_2)<d(v,x|G_2)}n_u(e|G_2)$$
$$=n_1PI_{v}^{(2)}(G_2)+n_1{n_2}^{2}(n_1-1)^{2}m_x(G_2)+2n_1n_2(n_1-1)\underline{N}\,.$$

Eq. (6) is obtained by adding the quantities S_1 and S_2. ■

Theorem 2.7 The revised Szeged index of the rooted product $G_1\{G_2\}$ is given by

$$Sz^*(G_1\{G_2\}) = n_2{}^2 Sz^*(G_1) + n_1 Sz^*(G_2) + \frac{1}{4} n_1 n_2{}^2 m_2 (n_1{}^2 - 1) \quad (7)$$
$$- \frac{1}{4} n_1 n_2{}^2 (n_1 - 1)^2 m_x(G_2) + \frac{1}{2} n_1 n_2 (n_1 - 1)(\overline{N} - \underline{N}) .$$

Proof. By Eq. (5),

$$Sz^*(G_1\{G_2\}) = \frac{1}{4}(m_1 + n_1 m_2)(n_1 n_2)^2 - \frac{1}{4} PI_v^{(2)}(G_1\{G_2\}) + \frac{1}{2} Sz(G_1\{G_2\}) .$$

By Eq. (1) and Eq. (6), we obtain

$$Sz^*(G_1\{G_2\}) = \frac{1}{4}(m_1 + n_1 m_2)(n_1 n_2)^2 - \frac{1}{4}[n_2{}^2 PI_v^{(2)}(G_1) + n_1 PI_v^{(2)}(G_2)$$
$$+ n_1 n_2{}^2 (n_1 - 1)^2 m_x(G_2) + 2 n_1 n_2 (n_1 - 1)\underline{N}]$$
$$+ \frac{1}{2}[n_2{}^2 Sz(G_1) + n_1 Sz(G_2) + n_1 n_2 (n_1 - 1)\overline{N}] .$$

Eq. (7) is obtained by simplifying the above expression. ■

3. Examples and corollaries

In this section, we apply Eqs. (1)-(4) and Eq. (7) to compute the Szeged index, vertex PI index, weighted Szeged index, weighted vertex PI index, and revised Szeged index of some chemical graphs.

Table 1

Some topological indices of path, star, and cycle

Graph	P_n	S_n	C_n, *n is even*	C_n, *n is odd*
Sz	$\binom{n+1}{3}$	$(n-1)^2$	$\frac{n^3}{4}$	$\frac{n(n-1)^2}{4}$
PI_v	$n(n-1)$	$n(n-1)$	n^2	$n(n-1)$
Sz_w	$\frac{2}{3}(n-1)(n^2+n-3)$	$n(n-1)^2$	n^3	$n(n-1)^2$
PI_w	$n(4n-6)$	$n^2(n-1)$	$4n^2$	$4n(n-1)$
Sz^*	$\binom{n+1}{3}$	$(n-1)^2$	$\frac{n^3}{4}$	$\frac{n^3}{4}$

Let P_n, S_n, and C_n denote the *n*-vertex path, star, and cycle, respectively. Throughout this section, we assume that P_n is rooted at one of its pendant vertices (vertices of degree one) and S_n is rooted at its vertex of degree $n-1$. Because of symmetry of C_n any vertex of this graph can be considered at its root vertex. Some topological indices of these graphs have been given in Table 1.

As the first example, consider the rooted product of P_n and P_m. This molecular graph is called the *comb lattice graph*. Using Eqs. (1)-(4), Eq. (7), and Table 1, we easily arrive at:

Corollary 3.1 Let $G = P_n\{P_m\}$. The following equalities hold.

(i) $Sz(G) = \frac{nm^3}{6}(3n-2) + \frac{nm^2}{6}(n-1)(n-2) - \frac{nm}{6}$;

(ii) $PI_v(G) = nm(nm-1)$;

(iii) $Sz_w(G) = \begin{cases} \frac{2nm^3}{3}(3n-2) + m^2(n^2-4)(n-1) - \frac{2m}{3}(3n^2-5n+6) + 2 & m \neq 2, \\ 4n^3 + 12n^2 - 24n + 10 & m = 2; \end{cases}$

(iv) $PI_w(G) = 4n^2m^2 + 2nm(n-5)$;

(v) $Sz^*(G) = \frac{nm^3}{6}(3n-2) + m^2\binom{n}{3} - \frac{nm}{6}$.

Let $P_n^*(m)$ denote the *m-thorn path* which is the graph obtained by attaching m pendant vertices to each vertex of the path P_n. This graph can be viewed as the rooted product of P_n and the star graph on $m+1$ vertices S_{m+1}. Using Eqs. (1)-(4), Eq. (7), and Table 1, we easily arrive at:

Corollary 3.2 The following equalities hold.

(i) $Sz(P_n^*(m)) = \frac{nm^2}{6}(n^2+6n-1) + \frac{nm}{3}(n-1)(n+4) + \binom{n}{3}$;

(ii) $PI_v(P_n^*(m)) = n(m+1)(nm+n-1)$;

(iii) $Sz_w(P_n^*(m)) = \frac{nm^3}{3}(n^2+3n-1) + \frac{m^2}{3}(4n^3+12n^2-19n+6)$
$+ \frac{m}{3}(5n^3+9n^2-32n+18) + \frac{2}{3}(n^3-4n+3)$;

(iv) $PI_w(P_n^*(m)) = n^2m^3 + 2nm^2(3n-2) + nm(9n-10) + 2n(n-3)$;

(v) $Sz^*(P_n^*(m)) = \frac{nm^2}{6}(n^2+6n-1) + \frac{nm}{3}(n-1)(n+4) + \binom{n}{3}$.

Let $C_n^*(m)$ denote the *m-thorn cycle* which is the graph obtained by attaching m pendant vertices to each vertex of the cycle C_n. This graph can be seen as the rooted product of C_n and the star graph on $m+1$ vertices S_{m+1}. Using Eqs. (1)-(4), Eq. (7), and Table 1, we easily arrive at:

Corollary 3.3 The following equalities hold.

(i) $Sz(C_n^*(m)) = \begin{cases} \frac{n^2m^2}{4}(n+4) + \frac{nm}{2}(n^2+2n-2) + \frac{n^3}{4} & n \text{ is even}, \\ \frac{nm^2}{4}(n+1)^2 + \frac{nm}{4}(n^2-1) + \frac{n}{4}(n-1)^2 & n \text{ is odd}; \end{cases}$

(ii) $PI_v(C_n^*(m)) = \begin{cases} n^2(m+1)^2 & n \text{ is even}, \\ n(m+1)(nm+n-1) & n \text{ is odd}; \end{cases}$

(iii) $Sz_w(C_n^*(m)) = \begin{cases} \frac{n^2m^3}{2}(n+2) + nm^2(2n^2+4n-1) & n \text{ is even} \\ +\frac{nm}{2}(5n^2+6n-6) + n^3, & \\ \frac{nm^3}{2}(n^2+1) + nm^2(2n^2+1) & n \text{ is odd} \\ +\frac{nm}{2}(5n^2-4n-1) + n(n-1)^2; & \end{cases}$

(iv) $PI_w(C_n^*(m)) = \begin{cases} n^2(m+1)^2(m+4) & n \text{ is even}, \\ n^2m^3 + 2nm^2(3n-1) + 3nm(3n-2) + 4n(n-1) & n \text{ is odd}; \end{cases}$

(v) $Sz^*(C_n^*(m)) = \frac{n^2m^2}{4}(n+4) + \frac{nm}{2}(n^2+2n-2) + \frac{n^3}{4}$.

Finally, consider the rooted product of P_n and C_m. Using Eqs. (1)-(4), Eq. (7), and Table 1, we easily arrive at:

Corollary 3.4 Let $G = P_n\{C_m\}$. The following equalities hold.

(i) $Sz(G) = \begin{cases} \frac{nm^3}{4}(2n-1) + m^2\binom{n+1}{3} & m \text{ is even}, \\ \frac{nm^3}{4}(2n-1) + \frac{nm^2}{6}(n^2-6n+2) + \frac{nm}{4}(2n-1) & m \text{ is odd}; \end{cases}$

(ii) $PI_v(G) = \begin{cases} nm(nm+n-1) & m \text{ is even}, \\ nm(nm-1) & m \text{ is odd}; \end{cases}$

(iii) $Sz_w(G) = \begin{cases} nm^3(2n-1) + \frac{m^2}{3}(4n^3+6n^2-19n+9) & m \text{ is even}, \\ nm^3(2n-1) + \frac{m^2}{3}(4n^3-6n^2-13n+9) + n(m+1) - 1 & m \text{ is odd}; \end{cases}$

(iv) $PI_w(G)=\begin{cases}4n^2m^2+2nm(6n-7) & m \text{ is even},\\ 4n^2m^2+2nm(4n-7)-4(n-1) & m \text{ is odd};\end{cases}$

(v) $Sz^*(G)=\begin{cases}\dfrac{nm^3}{4}(2n-1)+m^2\dbinom{n+1}{3} & m \text{ is even},\\ \dfrac{nm^3}{4}(2n-1)+\dfrac{nm^2}{12}(5n-1)(n-1) & m \text{ is odd}.\end{cases}$

R E F E R E N C E S

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