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On the Zagreb and Eccentricity Coindices of Graph Products

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Abstract. The second Zagreb coindex is a well-known graph invariant defined as the total degree product of all non-adjacent vertex pairs in a graph. The second Zagreb eccentricity coindex is defined analogously to the second Zagreb coindex by replacing the vertex degrees with the vertex eccentricities. In this paper, we present exact expressions or sharp lower bounds for the second Zagreb eccentricity coindex of some graph products such as lexicographic product, generalized hierarchical product, and strong product. Results are applied to compute the values of this eccentricity-based invariant for some chemical graphs and nanostructures such as hexagonal chain, linear phenylene chain, and zig-zag polyhex nanotube.

Keywords: Eccentricity of a vertex, Graph invariants, Graph products, Chemical graphs.

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1. Introduction

All graphs considered in this paper are finite, simple and connected. Let G be a graph on n vertices and m edges. We denote the vertex set and edge set of G by $V(G)$ and $E(G)$, respectively. The degree $d_G(u)$ of a vertex $u \in V(G)$ is the number of edges incident to u. The distance $d_G(u, v)$ between the vertices

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$u, v \in V(G)$ is defined as the length of any shortest path in G connecting u and v. The eccentricity $\varepsilon_G(u)$ of a vertex $u \in V(G)$ is the largest distance between u and any other vertex v of G, i.e., $\varepsilon_G(u) = \max_{v \in V(G)} d_G(u, v)$. The diameter $d(G)$ (radius $r(G)$, resp.) of G is the maximum (minimum, resp.) eccentricity over all vertices of G. A graph G is called a self-centered graph if all of its vertices have a same eccentricity. A vertex $u \in V(G)$ is called a universal vertex if u is adjacent to every other vertex of G, i.e., $d_G(u) = n - 1$. We denote the number of universal vertices of G by $n_{n-1}(G)$.

In graph theory, an *invariant* is a property of graphs that depends only on its abstract structure, not on graph representations such as particular labeling or drawing of the graph. Such quantities are also called *topological indices*. In organic chemistry, topological indices have been found to be useful in chemical documentation, isomer discrimination, quantitative structure-property and structure-activity relationships (QSPR and QSAR), and pharmaceutical drug design [11]. Topological indices have gained considerable popularity and many new topological indices have been suggested and investigated in the mathematical chemistry literature in recent years.

The *Zagreb indices* were introduced by Gutman and Trinajstić [17] and Gutman *et al.* [16] more than forty years ago. These indices have since been used to study molecular complexity, chirality, ZE-isomerism, and hetero-systems. The first Zagreb index $M_1(G)$ and second Zagreb index $M_2(G)$ of G are respectively defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2 = \sum_{uv \in E(G)} \big(d_G(u) + d_G(v)\big),$$

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

For more information on Zagreb indices, see the recent surveys [1, 9] and the references quoted therein.

The *Zagreb coindices* were introduced by Doslić [12] in 2008. The first Zagreb coindex $\overline{M}_1(G)$ and second Zagreb coindex $\overline{M}_2(G)$ of G are respectively defined as

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} \big(d_G(u) + d_G(v)\big), \ \overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u) d_G(v).$$

One may be referred to [4, 15, 19, 21, 23] for more details on Zagreb coindices.

The *eccentric connectivity index* was introduced by Sharma *et al.* [24] in 1997 as

$$\xi^c(G) = \sum_{u \in V(G)} d_G(u) \varepsilon_G(u) = \sum_{uv \in E(G)} \big(\varepsilon_G(u) + \varepsilon_G(v)\big).$$

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The eccentric connectivity index was successfully used for mathematical models of biological activities of diverse nature. Details on its mathematical theory and applications can be found in [3, 13, 14, 20].

The *total eccentricity* $\tau(G)$ of G is the sum of eccentricities of all vertices of G.

The *Zagreb eccentricity indices* were introduced by Vukičević and Graovac [26] analogously to Zagreb indices by replacing the vertex degrees with the vertex eccentricities. The first Zagreb eccentricity index $E_1(G)$ and second Zagreb eccentricity index $E_2(G)$ of G are respectively defined as

$$E_1(G) = \sum_{u \in V(G)} \varepsilon_G(u)^2, \ E_2(G) = \sum_{uv \in E(G)} \varepsilon_G(u)\varepsilon_G(v).$$

Some mathematical properties of these indices were investigated in [7, 10, 22].

Motivated by definition of Zagreb coindices, Hua and Miao [18] considered the total eccentricity sum of all non-adjacent vertex pairs of a graph and called this invariant the *eccentric connectivity coindex*. More formally, the eccentric connectivity coindex $\overline{\xi}^c(G)$ of G is defined as

$$\overline{\xi}^c(G) = \sum_{uv \notin E(G)} \big(\varepsilon_G(u) + \varepsilon_G(v)\big).$$

Motivated by definition of Zagreb coindices and eccentric connectivity coindex, the present author considered the total eccentricity product of all non-adjacent vertex pairs of a graph and called this eccentricity-based invariant the *second Zagreb eccentricity coindex* [6]. More formally, the second Zagreb eccentricity coindex $\overline{E}_2(G)$ of G is defined as

$$\overline{E}_2(G) = \sum_{uv \notin E(G)} \varepsilon_G(u)\varepsilon_G(v).$$

The present author investigated some basic mathematical properties of $\overline{E}_2$ and gave a comparison between $\overline{E}_2$ and $\overline{\xi}^c$ [6]. The extremal values of $\overline{E}_2$ over some special classes of graphs such as trees, unicyclic graphs, connected graphs, and connected bipartite graphs were also determined in [6]. In [5], several lower and upper bounds on $\overline{E}_2$ in terms of some graph parameters were obtained and the values of $\overline{E}_2$ for double graphs and extended double graphs were computed. In this paper, we study $\overline{E}_2$ under some graph products namely lexicographic product, generalized hierarchical product, and strong product and apply our results to compute the values of this invariant for some graphs of chemical interest by specializing components in graph products.

2. Main Results

In this section, we present exact expressions or sharp lower bounds for the second Zagreb eccentricity coindex of some graph products in terms of the respective indices of their components, the number of their vertices, the number

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of their edges, and in some cases also the number of their universal vertices. Let G_1 and G_2 denote the components of each graph product which are considered to be finite simple connected graphs. For a given component graph G_i, the number of vertices and edges are denoted by n_i and m_i, respectively, where $i = 1, 2$. The notation $\overline{m}_i$ is used for the number of edges of $\overline{G}_i$, which is equal to $\binom{n_i}{2} - m_i$, $i = 1, 2$. Further studies on topological invariants of graph products can be found in [2, 14, 25].

2.1. **Lexicographic product.** The *lexicographic product* $G_1[G_2]$ of graphs G_1 and G_2 is a graph with vertex set $V(G_1) \times V(G_2)$ and two vertices (u_1, u_2) and (v_1, v_2) are adjacent whenever $u_1v_1 \in E(G_1)$ or $[u_1 = v_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)]$. The lexicographic product of two graphs is also known as their *composition*. The eccentricity of a vertex (u_1, u_2) in $G_1[G_2]$ is given by

$$\varepsilon_{G_1[G_2]}((u_1,u_2)) = \begin{cases} 1 & \text{if } \varepsilon_{G_1}(u_1) = \varepsilon_{G_2}(u_2) = 1, \\ 2 & \text{if } \varepsilon_{G_1}(u_1) = 1,\ \varepsilon_{G_2}(u_2) \geq 2, \\ \varepsilon_{G_1}(u_1) & \text{if } \varepsilon_{G_1}(u_1) \geq 2. \end{cases}$$

Theorem 2.1. *The second Zagreb eccentricity coindex of $G_1[G_2]$ is given by*

$$\overline{E}_2(G_1[G_2]) = {n_2}^2\overline{E}_2(G_1) + \overline{m}_2\big(3n_{n_1-1}(G_1) + E_1(G_1)\big). \tag{2.1}$$

Proof. By definition of the second Zagreb eccentricity coindex, we obtain

$$\begin{aligned}
\overline{E}_2(G_1[G_2]) = & \sum_{(u_1,u_2)(v_1,v_2)\notin E(G_1[G_2])} \varepsilon_{G_1[G_2]}((u_1,u_2))\varepsilon_{G_1[G_2]}((v_1,v_2)) \\
= & \sum_{\substack{u_1\in V(G_1),\\ \varepsilon_{G_1}(u_1)=1}} \sum_{u_2v_2\notin E(G_2)} (2\times 2) + \sum_{\substack{u_1\in V(G_1),\\ \varepsilon_{G_1}(u_1)\geq 2}} \sum_{u_2v_2\notin E(G_2)} \varepsilon_{G_1}(u_1)^2 \\
& + \sum_{u_2\in V(G_2)} \sum_{u_1v_1\notin E(G_1)} \varepsilon_{G_1}(u_1)\varepsilon_{G_1}(v_1) \\
& + 2\sum_{u_1v_1\notin E(G_1)} \sum_{\{u_2,v_2\}\subseteq V(G_2)} \varepsilon_{G_1}(u_1)\varepsilon_{G_1}(v_1) \\
= & \overline{m}_2\big(4n_{n_1-1}(G_1) + E_1(G_1) - n_{n_1-1}(G_1)\big) + \Big(n_2 + 2\binom{n_2}{2}\Big)\overline{E}_2(G_1),
\end{aligned}$$

from which we straightforwardly arrive at Eq. (2.1). □

Corollary 2.2. *Let G_1 contain no universal vertices. Then*

$$\overline{E}_2(G_1[G_2]) = {n_2}^2\overline{E}_2(G_1) + \overline{m}_2E_1(G_1).$$

2.2. **Generalized hierarchical product.** Let $\phi \neq U \subseteq V(G_1)$. The *generalized hierarchical product* $G_1(U) \sqcap G_2$ of graphs G_1 and G_2 is a graph with vertex set $V(G_1)\times V(G_2)$ and vertices (u_1, u_2) and (v_1, v_2) are adjacent whenever $[u_1 = v_1 \in U$ and $u_2v_2 \in E(G_2)]$ or $[u_2 = v_2 \in V(G_2)$ and $u_1v_1 \in E(G_1)]$.

For $\phi \neq U \subseteq V(G)$, a path between vertices $u, v \in V(G)$ through U is a uv-path in G containing some vertex $z \in U$ (vertex z could be the vertex u or

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vertex v). The distance between u and v through U, denoted by $d_{G(U)}(u,v)$, is the length of any shortest path between u and v through U. Note that if one of the vertices u and v belongs to U, then $d_{G(U)}(u,v) = d_G(u,v)$. For $u \in V(G)$, we define $\varepsilon_{G(U)}(u) = \max_{v\in V(G)} d_{G(U)}(u,v)$. For notational convenience, we define some invariants related to U as follows:

$$\begin{aligned}
\tau(U) &= \sum_{u\in U} \varepsilon_{G(U)}(u) = \sum_{u\in U} \varepsilon_G(u);\\
E_1(U) &= \sum_{u\in U} \varepsilon_{G(U)}(u)^2 = \sum_{u\in U} \varepsilon_G(u)^2;\\
\tau(G(U)) &= \sum_{u\in V(G)} \varepsilon_{G(U)}(u);\\
E_1(G(U)) &= \sum_{u\in V(G)} \varepsilon_{G(U)}(u)^2;\\
\overline{\xi}^c(G(U)) &= \sum_{uv\notin E(G)} \big(\varepsilon_{G(U)}(u) + \varepsilon_{G(U)}(v)\big);\\
\overline{E}_2(G(U)) &= \sum_{uv\notin E(G)} \varepsilon_{G(U)}(u)\varepsilon_{G(U)}(v).
\end{aligned}$$

The eccentricity of a vertex (u_1,u_2) in $G_1(U) \sqcap G_2$ was given in [8],

$$\varepsilon_{G_1(U)\sqcap G_2}((u_1,u_2)) = \varepsilon_{G_1(U)}(u_1) + \varepsilon_{G_2}(u_2).$$

Theorem 2.3. *The second Zagreb eccentricity coindex of $G_1(U) \sqcap G_2$ is given by*

$$\begin{aligned}
\overline{E}_2(G_1(U) \sqcap G_2) =& n_2\overline{E}_2(G_1(U)) + |U|\overline{E}_2(G_2) - m_2E_1(U)\\
&- \frac{1}{2}(n_1 - |U| + 2m_1)E_1(G_2) + \binom{n_2}{2}\tau(G_1(U))^2\\
&+ \frac{1}{2}({n_1}^2 - |U|)\tau(G_2)^2 + \overline{\xi}^c(G_1(U))\tau(G_2) + \overline{\xi}^c(G_2)\tau(U)\\
&+ (n_2-1)\big(n_1\tau(G_1(U)) - \tau(U)\big)\tau(G_2).
\end{aligned} \tag{2.2}$$

Proof. By definition of the second Zagreb eccentricity coindex, we obtain

$$\overline{E}_2(G_1(U)\sqcap G_2) = \sum_{(u_1,u_2)(v_1,v_2)\notin E(G_1(U)\sqcap G_2)} \varepsilon_{G_1(U)\sqcap G_2}((u_1,u_2))\varepsilon_{G_1(U)\sqcap G_2}((v_1,v_2)).$$

We partition the above sum into four sums $S_1,\ S_2,\ S_3,\ S_4$ as follows.

The first sum S_1 is taken over all vertices $u_1 \in U$ and non-adjacent vertex pairs $u_2v_2 \notin E(G_2)$,

$$\begin{aligned}
S_1 =& \sum_{u_1\in U} \sum_{u_2v_2\notin E(G_2)} \big(\varepsilon_{G_1(U)}(u_1)+\varepsilon_{G_2}(u_2)\big)\big(\varepsilon_{G_1(U)}(u_1)+\varepsilon_{G_2}(v_2)\big)\\
=& \sum_{u_1\in U} \sum_{u_2v_2\notin E(G_2)} \big[\varepsilon_{G_1(U)}(u_1)^2+\big(\varepsilon_{G_2}(u_2)+\varepsilon_{G_2}(v_2)\big)\varepsilon_{G_1(U)}(u_1)\\
&+\varepsilon_{G_2}(u_2)\varepsilon_{G_2}(v_2)\big]\\
=&\overline{m}_2E_1(U)+\overline{\xi}^c(G_2)\tau(U)+|U|\overline{E}_2(G_2).
\end{aligned}$$

The second sum S_2 is taken over all vertices $u_2 \in V(G_2)$ and non-adjacent vertex pairs $u_1v_1 \notin E(G_1)$,

$$\begin{aligned}
S_2 =& \sum_{u_2\in V(G_2)} \sum_{u_1v_1\notin E(G_1)} \big(\varepsilon_{G_1(U)}(u_1)+\varepsilon_{G_2}(u_2)\big)\big(\varepsilon_{G_1(U)}(v_1)+\varepsilon_{G_2}(u_2)\big)\\
=& \sum_{u_2\in V(G_2)} \sum_{u_1v_1\notin E(G_1)} \big[\varepsilon_{G_2}(u_2)^2+\big(\varepsilon_{G_1(U)}(u_1)+\varepsilon_{G_1(U)}(v_1)\big)\varepsilon_{G_2}(u_2)\\
&+\varepsilon_{G_1(U)}(u_1)\varepsilon_{G_1(U)}(v_1)\big]\\
=&\overline{m}_1E_1(G_2)+\overline{\xi}^c(G_1(U))\tau(G_2)+n_2\overline{E}_2(G_1(U)).
\end{aligned}$$

The third sum S_3 is taken over all vertices $u_1 \in V(G_1)\setminus U$ and unordered vertex pairs $\{u_2, v_2\} \subseteq V(G_2)$,

$$\begin{aligned}
S_3 =& \sum_{u_1\in V(G_1)\setminus U} \sum_{\{u_2,v_2\}\subseteq V(G_2)} \big(\varepsilon_{G_1(U)}(u_1)+\varepsilon_{G_2}(u_2)\big)\big(\varepsilon_{G_1(U)}(u_1)+\varepsilon_{G_2}(v_2)\big)\\
=& \sum_{u_1\in V(G_1)\setminus U} \sum_{\{u_2,v_2\}\subseteq V(G_2)} \big[\varepsilon_{G_1(U)}(u_1)^2+\big(\varepsilon_{G_2}(u_2)+\varepsilon_{G_2}(v_2)\big)\varepsilon_{G_1(U)}(u_1)\\
&+\varepsilon_{G_2}(u_2)\varepsilon_{G_2}(v_2)\big]\\
=&\binom{n_2}{2}\big[E_1(G_1(U))-E_1(U)\big]+\big[\tau(G_1(U)-\tau(U)\big](n_2-1)\tau(G_2)\\
&+\frac{1}{2}(n_1-|U|)\big[\tau(G_2)^2-E_1(G_2)\big].
\end{aligned}$$

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The fourth sum S_4 is taken over all unordered vertex pairs $\{u_1, v_1\} \subseteq V(G_1)$ and $\{u_2, v_2\} \subseteq V(G_2)$,

$$\begin{aligned}
S_4 = &\sum_{\{u_1,v_1\}\subseteq V(G_1)} \sum_{\{u_2,v_2\}\subseteq V(G_2)} \Big[\big(\varepsilon_{G_1(U)}(u_1) + \varepsilon_{G_2}(u_2)\big)\big(\varepsilon_{G_1(U)}(v_1) + \varepsilon_{G_2}(v_2)\big) \\
&+ \big(\varepsilon_{G_1(U)}(u_1) + \varepsilon_{G_2}(v_2)\big)\big(\varepsilon_{G_1(U)}(v_1) + \varepsilon_{G_2}(u_2)\big)\Big] \\
= &\sum_{\{u_1,v_1\}\subseteq V(G_1)} \sum_{\{u_2,v_2\}\subseteq V(G_2)} \Big[2\varepsilon_{G_1(U)}(u_1)\varepsilon_{G_1(U)}(v_1) + 2\varepsilon_{G_2}(u_2)\varepsilon_{G_2}(v_2) \\
&+ \big(\varepsilon_{G_1(U)}(u_1) + \varepsilon_{G_1(U)}(v_1)\big)\big(\varepsilon_{G_2}(u_2) + \varepsilon_{G_2}(v_2)\big)\Big] \\
= &\binom{n_2}{2}\big[\tau(G_1(U))^2 - E_1(G_1(U))\big] + \binom{n_1}{2}\big[\tau(G_2)^2 - E_1(G_2)\big] \\
&+ (n_1 - 1)(n_2 - 1)\tau(G_1(U))\tau(G_2).
\end{aligned}$$

Eq. (2.2) now follows by adding the quantities $S_1,\ S_2,\ S_3,\ S_4$ and simplifying the resulting expression. □

The *Cartesian product* $G_1 \square G_2$ of graphs G_1 and G_2 is a graph with vertex set $V(G_1) \times V(G_2)$ and two vertices (u_1, u_2) and (v_1, v_2) are adjacent whenever $[u_1 = v_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)]$ or $[u_2 = v_2 \in V(G_2)$ and $u_1v_1 \in E(G_1)]$. Note that if $U = V(G_1)$, then $G_1 \square G_2 = G_1(U) \sqcap G_2$ and by Theorem 2.3, we get the following corollary.

Corollary 2.4. *The second Zagreb eccentricity coindex of $G_1 \square G_2$ is given by*

$$\begin{aligned}
\overline{E}_2(G_1 \square G_2) = &n_2\overline{E}_2(G_1) + n_1\overline{E}_2(G_2) - m_2E_1(G_1) - m_1E_1(G_2) \\
&+ \binom{n_2}{2}\tau(G_1)^2 + \binom{n_1}{2}\tau(G_2)^2 + \overline{\xi}^c(G_1)\tau(G_2) \\
&+ \overline{\xi}^c(G_2)\tau(G_1) + (n_1 - 1)(n_2 - 1)\tau(G_1)\tau(G_2).
\end{aligned}$$

2.3. **Strong product.** The *strong product* $G_1 \boxtimes G_2$ of graphs G_1 and G_2 is a graph with vertex set $V(G_1) \times V(G_2)$ and two vertices (u_1, u_2) and (v_1, v_2) are adjacent whenever $[u_1 = v_1 \in V(G_1)$ and $u_2v_2 \in E(G_2)]$ or $[u_2 = v_2 \in V(G_2)$ and $u_1v_1 \in E(G_1)]$ or $[u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)]$. The eccentricity of a vertex (u_1, u_2) of $G_1 \boxtimes G_2$ was given in [25],

$$\varepsilon_{G_1 \boxtimes G_2}((u_1, u_2)) = \max\{\varepsilon_{G_1}(u_1), \varepsilon_{G_2}(u_2)\}.$$

In the following theorem, we give a lower bound on the second Zagreb eccentricity coindex of $G_1 \boxtimes G_2$.

Theorem 2.5. *The second Zagreb eccentricity coindex of $G_1 \boxtimes G_2$ is given by*

$$\begin{aligned}
\overline{E}_2(G_1 \boxtimes G_2) \geq &\frac{1}{4}\big[(n_2 + 2m_2)\overline{E}_2(G_1) + (n_1 + 2m_1)\overline{E}_2(G_2) + \overline{m}_2\tau(G_1)^2 \\
&+ \overline{m}_1\tau(G_2)^2 + \big(\tau(G_2) + \xi^c(G_2)\big)\overline{\xi}^c(G_1) \\
&+ \big(\tau(G_1) + \xi^c(G_1)\big)\overline{\xi}^c(G_2) + \overline{\xi}^c(G_1)\overline{\xi}^c(G_2)\big].
\end{aligned} \tag{2.3}$$

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The equality holds in (2.3) if and only if G_1 and G_2 are self-centered graphs and $d(G_1) = d(G_2)$.

Proof. It is a well-known fact that for each pair of real numbers a, b, we have $max\{a, b\} \geq \frac{a+b}{2}$, with equality if and only if $a = b$. Now by definition of the second Zagreb eccentricity coindex, we obtain

$$\begin{aligned}
\overline{E}_2(G_1 \boxtimes G_2) &= \sum_{(u_1,u_2)(v_1,v_2)\notin E(G_1\boxtimes G_2)} \varepsilon_{G_1\boxtimes G_2}((u_1,u_2))\varepsilon_{G_1\boxtimes G_2}((v_1,v_2)) \\
&= \sum_{(u_1,u_2)(v_1,v_2)\notin E(G_1\boxtimes G_2)} \max\{\varepsilon_{G_1}(u_1), \varepsilon_{G_2}(u_2)\} \\
&\quad \times \max\{\varepsilon_{G_1}(v_1), \varepsilon_{G_2}(v_2)\} \\
&\geq \sum_{(u_1,u_2)(v_1,v_2)\notin E(G_1\boxtimes G_2)} \frac{\varepsilon_{G_1}(u_1) + \varepsilon_{G_2}(u_2)}{2} \times \frac{\varepsilon_{G_1}(v_1) + \varepsilon_{G_2}(v_2)}{2},
\end{aligned}$$

from which we arrive at

$$\overline{E}_2(G_1\boxtimes G_2) \geq \frac{1}{4} \sum_{(u_1,u_2)(v_1,v_2)\notin E(G_1\boxtimes G_2)} \big(\varepsilon_{G_1}(u_1)+\varepsilon_{G_2}(u_2)\big)\big(\varepsilon_{G_1}(v_1)+\varepsilon_{G_2}(v_2)\big). \tag{2.4}$$

The right hand side expression in (2.4) can be partitioned into four sums $S_1,\ S_2,\ S_3,\ S_4$ as follows.

The first sum S_1 is taken over all vertices $u_1 \in V(G_1)$ and non-adjacent vertex pairs $u_2v_2 \notin E(G_2)$,

$$\begin{aligned}
S_1 =& \frac{1}{4} \sum_{u_1\in V(G_1)} \sum_{u_2v_2\notin E(G_2)} \big(\varepsilon_{G_1}(u_1) + \varepsilon_{G_2}(u_2)\big)\big(\varepsilon_{G_1}(u_1) + \varepsilon_{G_2}(v_2)\big) \\
=& \frac{1}{4} \sum_{u_1\in V(G_1)} \sum_{u_2v_2\notin E(G_2)} [\varepsilon_{G_1}(u_1)^2 + \big(\varepsilon_{G_2}(u_2) + \varepsilon_{G_2}(v_2)\big)\varepsilon_{G_1}(u_1) \\
&+ \varepsilon_{G_2}(u_2)\varepsilon_{G_2}(v_2)] \\
=& \frac{1}{4}\big[\overline{m}_2 E_1(G_1) + \tau(G_1)\overline{\xi}^c(G_2) + n_1\overline{E}_2(G_2)\big].
\end{aligned}$$

The second sum S_2 is taken over all vertices $u_2 \in V(G_2)$ and non-adjacent vertex pairs $u_1v_1 \notin E(G_1)$,

$$S_2 = \frac{1}{4} \sum_{u_2\in V(G_2)} \sum_{u_1v_1\notin E(G_1)} \big(\varepsilon_{G_1}(u_1) + \varepsilon_{G_2}(u_2)\big)\big(\varepsilon_{G_1}(v_1) + \varepsilon_{G_2}(u_2)\big).$$

By symmetry, we obtain

$$S_2 = \frac{1}{4}\big[\overline{m}_1 E_1(G_2) + \tau(G_2)\overline{\xi}^c(G_1) + n_2\overline{E}_2(G_1)\big].$$

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The third sum S_3 is taken over all edges $u_1v_1 \in E(G_1)$ and non-adjacent vertex pairs $u_2v_2 \notin E(G_2)$,

$$\begin{aligned}S_3 =& \frac{1}{4}\sum_{u_1v_1\in E(G_1)}\sum_{u_2v_2\notin E(G_2)}\big[\big(\varepsilon_{G_1}(u_1)+\varepsilon_{G_2}(u_2)\big)\big(\varepsilon_{G_1}(v_1)+\varepsilon_{G_2}(v_2)\big)\\ &+\big(\varepsilon_{G_1}(u_1)+\varepsilon_{G_2}(v_2)\big)\big(\varepsilon_{G_1}(v_1)+\varepsilon_{G_2}(u_2)\big)\big]\\ =&\frac{1}{4}\sum_{u_1v_1\in E(G_1)}\sum_{u_2v_2\notin E(G_2)}\big[2\varepsilon_{G_1}(u_1)\varepsilon_{G_1}(v_1)+2\varepsilon_{G_2}(u_2)\varepsilon_{G_2}(v_2)\\ &+\big(\varepsilon_{G_1}(u_1)+\varepsilon_{G_1}(v_1)\big)\big(\varepsilon_{G_2}(u_2)+\varepsilon_{G_2}(v_2)\big)\big]\\ =&\frac{1}{4}\big[2\overline{m}_2E_2(G_1)+2m_1\overline{E}_2(G_2)+\xi^c(G_1)\overline{\xi}^c(G_2)\big].\end{aligned}$$

The fourth sum S_4 is taken over all non-adjacent vertex pairs $u_1v_1 \notin E(G_1)$ and unordered vertex pairs $\{u_2, v_2\} \subseteq V(G_2)$,

$$\begin{aligned}S_4 =& \frac{1}{4}\sum_{u_1v_1\notin E(G_1)}\sum_{\{u_2,v_2\}\subseteq V(G_2)}\big[\big(\varepsilon_{G_1}(u_1)+\varepsilon_{G_2}(u_2)\big)\big(\varepsilon_{G_1}(v_1)+\varepsilon_{G_2}(v_2)\big)\\ &+\big(\varepsilon_{G_1}(u_1)+\varepsilon_{G_2}(v_2)\big)\big(\varepsilon_{G_1}(v_1)+\varepsilon_{G_2}(u_2)\big)\big]\\ =&\frac{1}{4}\sum_{u_1v_1\notin E(G_1)}\sum_{\{u_2,v_2\}\subseteq V(G_2)}\big[2\varepsilon_{G_1}(u_1)\varepsilon_{G_1}(v_1)+2\varepsilon_{G_2}(u_2)\varepsilon_{G_2}(v_2)\\ &+\big(\varepsilon_{G_1}(u_1)+\varepsilon_{G_1}(v_1)\big)\big(\varepsilon_{G_2}(u_2)+\varepsilon_{G_2}(v_2)\big]\\ =&\frac{1}{4}\big[2\binom{n_2}{2}\overline{E}_2(G_1)+2\overline{m}_1\big(E_2(G_2)+\overline{E}_2(G_2)\big)+\overline{\xi}^c(G_1)\big(\xi^c(G_2)+\overline{\xi}^c(G_2)\big)\big].\end{aligned}$$

The inequality in (2.3) now follows from Eq. (2.4) by adding the quantities $S_1,\ S_2,\ S_3,\ S_4$ and simplifying the resulting expression.

The equality holds in (2.3) if and only if for each $(u_1, u_2)(v_1, v_2) \notin E(G_1 \boxtimes G_2)$, $\varepsilon_{G_1}(u_1) = \varepsilon_{G_1}(u_2)$ and $\varepsilon_{G_2}(v_1) = \varepsilon_{G_2}(v_2)$. If G_1 and G_2 are self-centered graphs and $d(G_1) = d(G_2)$, then the equality in (2.3) holds trivially. Now let the equality hold in (2.3). Then for each $u_1 \in V(G_1)$, $u_2v_2 \notin E(G_2)$, $\varepsilon_{G_1}(u_1) = \varepsilon_{G_2}(u_2) = \varepsilon_{G_2}(v_2)$, and for each $u_2 \in V(G_2)$, $u_1v_1 \notin E(G_1)$, $\varepsilon_{G_2}(u_2) = \varepsilon_{G_1}(u_1) = \varepsilon_{G_1}(v_1)$. This implies that G_1 and G_2 are self-centered graphs and $d(G_1) = d(G_2)$. □

If the radios of one of the component in strong product is greater than or equal to the diameter of the other component, we can obtain an exact formula for $\overline{E}_2(G_1 \boxtimes G_2)$.

Theorem 2.6. *Let $r(G_1) \geq d(G_2)$. The second Zagreb eccentricity coindex of $G_1 \boxtimes G_2$ is given by*

$$\overline{E}_2(G_1 \boxtimes G_2) = (n_2 + 2m_2)\overline{E}_2(G_1) + \overline{m}_2\tau(G_1)^2. \tag{2.5}$$

Proof. Under the condition $r(G_1) \geq d(G_2)$, for every vertex $u_1 \in V(G_1)$, $u_2 \in V(G_2)$, $\varepsilon_{G_1}(u_1) \geq \varepsilon_{G_2}(u_2)$, so $\varepsilon_{G_1 \boxtimes G_2}((u_1,u_2)) = \varepsilon_{G_1}(u_1)$. Now by definition of the second Zagreb eccentricity coindex, we have

$$\begin{aligned}
\overline{E}_2(G_1 \boxtimes G_2) = & \sum_{(u_1,u_2)(v_1,v_2)\notin E(G_1\boxtimes G_2)} \varepsilon_{G_1\boxtimes G_2}((u_1,u_2))\varepsilon_{G_1\boxtimes G_2}((v_1,v_2)) \\
= & \sum_{u_1\in V(G_1)} \sum_{u_2v_2\notin E(G_2)} \varepsilon_{G_1}(u_1)^2 \\
& + \sum_{u_2\in V(G_2)} \sum_{u_1v_1\notin E(G_1)} \varepsilon_{G_1}(u_1)\varepsilon_{G_1}(v_1) \\
& + 2 \sum_{u_1v_1\in E(G_1)} \sum_{u_2v_2\notin E(G_2)} \varepsilon_{G_1}(u_1)\varepsilon_{G_1}(v_1) \\
& + 2 \sum_{u_1v_1\notin E(G_1)} \sum_{\{u_2,v_2\}\subseteq V(G_2)} \varepsilon_{G_1}(u_1)\varepsilon_{G_1}(v_1) \\
= & \overline{m}_2 E_1(G_1) + n_2\overline{E}_2(G_1) + 2\overline{m}_2 E_2(G_1) + 2\binom{n_2}{2}\overline{E}_2(G_1) \\
= & {n_2}^2\overline{E}_2(G_1) + \overline{m}_2\big(E_1(G_1) + 2E_2(G_1)\big).
\end{aligned}$$

Eq. (2.5) now follows by plugging the expression $E_1(G_1)+2E_2(G_1) = \tau(G_1)^2 - 2\overline{E}_2(G_1)$ from [6] into the above formula and simplifying the resulting expression. □

3. Examples and applications

In this section, we apply the results obtained in Section 2 to compute the second Zagreb eccentricity coindex of some classes of chemically interesting graphs by specializing components in graph products.

The following results for path and cycle on n vertices follow easily by direct calculations and the proofs are therefore omitted.

Lemma 3.1. *The following hold:*

(i) $\tau(P_n) = \begin{cases} \frac{1}{4}(n-1)(3n+1) & 2 \nmid n, \\ \frac{1}{4}n(3n-2) & 2 \mid n; \end{cases}$

(ii) $\xi^c(P_n) = \begin{cases} \frac{3}{2}(n-1)^2 & 2 \nmid n, \\ \frac{1}{2}(3n^2-6n+4) & 2 \mid n; \end{cases}$

(iii) $E_1(P_n) = \begin{cases} \frac{1}{12}(n-1)(7n^2-2n-3) & 2 \nmid n, \\ \frac{1}{12}n(n-1)(7n-2) & 2 \mid n; \end{cases}$

(iv) $E_2(P_n) = \begin{cases} \frac{1}{12}(n-1)(7n^2-14n+3) & 2 \nmid n, \\ \frac{1}{12}n(7n^2-21n+20) & 2 \mid n; \end{cases}$

(v) $\overline{\xi}^c(P_n) = \begin{cases} \frac{1}{4}(n-1)^2(3n-5) & 2 \nmid n, \\ \frac{1}{4}(n-2)(3n^2-5n+4) & 2 \mid n; \end{cases}$

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(vi) $\overline{E}_2(P_n) = \begin{cases} \frac{1}{32}(n-1)(9n^3-31n^2+35n-5) & 2\nmid n, \\ \frac{1}{32}n(n-2)(9n^2-22n+28) & 2\mid n. \end{cases}$

Lemma 3.2. *The following hold:*

(i) $\tau(C_n) = n\lfloor \frac{n}{2} \rfloor$;

(ii) $\xi^c(C_n) = 2n\lfloor \frac{n}{2} \rfloor$;

(iii) $E_1(C_n) = E_2(C_n) = n\lfloor \frac{n}{2} \rfloor^2$;

(iv) $\overline{\xi}^c(C_n) = n(n-3)\lfloor \frac{n}{2} \rfloor$;

(v) $\overline{E}_2(C_n) = \frac{1}{2}n(n-3)\lfloor \frac{n}{2} \rfloor^2$.

We start with some examples for lexicographic product. An *open fence* is lexicographic product of P_n and P_2 and a *closed fence* is lexicographic product of C_n and P_2. Using Theorem 2.1 and Lemmas 3.1 and 3.2, we arrive at:

Corollary 3.3.

$$\overline{E}_2(P_n[P_2]) = \begin{cases} \frac{1}{16}(n-1)(9n^3-31n^2+35n-5) & 2\nmid n, \\ \frac{n}{16}(n-2)(9n^2-22n+28) & 2\mid n; \end{cases}$$

$$\overline{E}_2(C_n[P_2]) = n(n-3)\lfloor \frac{n}{2} \rfloor^2.$$

Now, we consider some applications of generalized hierarchical product. The *hexagonal chain* L_n including n hexagons is the generalized hierarchical product $P_{2n+1}(U)\sqcap P_2$, where $U = \{v_{2k+1} : 0 \leq k \leq n\}$. Using Theorem 2.3 and Lemma 3.1, the second Zagreb eccentricity coindex of this graph is given by

Corollary 3.4.

$$\overline{E}_2(L_n) = \begin{cases} \frac{1}{3}(54n^4+95n^3+45n^2+n-3) & 2\nmid n, \\ \frac{n}{3}(54n^3+95n^2+45n+4) & 2\mid n. \end{cases}$$

The *zig-zag polyhex nanotube* $TUHC_6[2n,2]$ is the generalized hierarchical product $C_{2n}(U)\sqcap P_2$, where $U = \{v_{2k} : 1 \leq k \leq n\}$. Application of Theorem 2.3 and Lemmas 3.1 and 3.2 yields:

Corollary 3.5.

$$\overline{E}_2(TUHC_6[2n,2]) = n(8n^3+9n^2-6n-7).$$

The *linear phenylene chain* PH_n including n benzene rings is the generalized hierarchical product $P_{3n}(U)\sqcap P_2$, where $U = \{v_{3k+1} : 0 \leq k \leq n-1\} \cup \{v_{3k} : 1 \leq k \leq n\}$. Using Theorem 2.3 and Lemma 3.1, we obtain:

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Corollary 3.6.

$$\overline{E}_2(PH_n) = \begin{cases} \frac{1}{8}(729n^4 - 138n^3 - 72n^2 - 2n - 5) & 2 \nmid n, \\ \frac{1}{8}(729n^4 - 138n^3 - 18n^2 + 4n - 16) & 2 \mid n. \end{cases}$$

Now, we present some examples for strong product. Application of Theorem 2.6 yields:

Corollary 3.7. *For any graph G,*

$$\overline{E}_2(G \boxtimes K_m) = m^2\overline{E}_2(G).$$

By setting $G = P_n$ and $G = C_n$ in Corollary 3.7 and using Lemmas 3.1 and 3.2, we arrive at:

Corollary 3.8.

$$\overline{E}_2(P_n \boxtimes K_m) = \begin{cases} \frac{1}{32}m^2(n-1)(9n^3 - 31n^2 + 35n - 5) & 2 \nmid n, \\ \frac{1}{32}m^2 n(n-2)(9n^2 - 22n + 28) & 2 \mid n; \end{cases}$$
$$\overline{E}_2(C_n \boxtimes K_m) = \frac{1}{2}m^2 n(n-3)\lfloor\frac{n}{2}\rfloor^2.$$

Using Theorem 2.6, we also get the following corollary.

Corollary 3.9. *Let G be a graph of order m without universal vertices. Then*

$$\overline{E}_2(G \boxtimes K_{n_1,n_2,\ldots,n_r}) = (n^2 - n^{(2)} + n)\overline{E}_2(G) + \frac{1}{2}(n^{(2)} - n)\tau(G)^2,$$

where $n = n_1 + n_2 + \ldots + n_r$, $n^{(2)} = {n_1}^2 + {n_2}^2 + \ldots + {n_r}^2$.

By setting $G = P_m$ and $G = C_m$ in Corollary 3.9 and using Lemmas 3.1 and 3.2, we obtain:

Corollary 3.10. *For $m > 3$,*

$$\overline{E}_2(P_m \boxtimes K_{n_1,n_2,\ldots,n_r}) = \begin{cases} \frac{1}{32}(m-1)\big[4(n^{(2)} - n)(7m^2 - 10m + 1) & 2 \nmid m, \\ +n^2(9m^3 - 31m^2 + 35m - 5)\big] & \\ \frac{m}{32}\big[4(n^{(2)} - n)(7m^2 - 17m + 14) & 2 \mid m; \\ +n^2(9m^3 - 40m^2 + 72m - 56)\big] & \end{cases}$$
$$\overline{E}_2(C_m \boxtimes K_{n_1,n_2,\ldots,n_r}) = \frac{m}{2}\lfloor\frac{m}{2}\rfloor^2\big[3(n^{(2)} - n) + n^2(m-3)\big],$$

where $n = n_1 + n_2 + \ldots + n_r$, $n^{(2)} = {n_1}^2 + {n_2}^2 + \ldots + {n_r}^2$.

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