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THE WIENER, ECCENTRIC CONNECTIVITY AND ZAGREB INDICES OF THE HIERARCHICAL PRODUCT OF GRAPHS*

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Abstract. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs having a distinguished or root vertex, labeled 0. The hierarchical product $G_2 \sqcap G_1$ of G_2 and G_1 is a graph with vertex set $V_2 \times V_1$. Two vertices y_2y_1 and x_2x_1 are adjacent if and only if $y_1x_1 \in E_1$ and $y_2 = x_2$; or $y_2x_2 \in E_2$ and $y_1 = x_1 = 0$. In this paper, the Wiener, eccentric connectivity and Zagreb indices of this new operation of graphs are computed. As an application, these topological indices for a class of alkanes are computed.

1. Introduction. Throughout this paper by the word graph we mean a finite, undirected graph without loops or multiple edges. If two vertices a and b are adjacent then we use the notation $a \sim b$. A graph invariant or topological index is any function on a graph that does not depend on a labeling of its vertices.

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The distance between two vertices u and v of a graph G is denoted by $d_G(u,v)$ ($d(u,v)$ for short). It is defined as the number of edges in a minimum path connecting them. A distance-based topological index is one that is related to the above distance function. The first index is the well-known Wiener index [23] defined as the sum of all distances between vertices of a given graph G.

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. For every vertex $u \in V(G)$, the edge connecting u and v is denoted by uv and $deg_G(u)$ denotes the degree of u in G. The diameter of G, $diam_G(G)$, is the maximum possible distance between any two vertices in the graph. We will omit the subscript G when the graph is clear from the context.

The first and second Zagreb indices [12, 13, 19] were originally defined as

$$M_1(G) = \sum_{u \in V(G)} deg(u)^2$$

and

$$M_2(G) = \sum_{uv \in E(G)} deg(u)deg(v),$$

respectively. These topological indices have numerous applications in chemistry and attracted significant attention from mathematicians [11, 16]. The Zagreb indices can be viewed as the contributions of pairs of adjacent vertices to certain degree-weighted generalizations of Wiener polynomials [9]. It turned out that computing such polynomials for certain composite graphs depends on such contributions from pairs of non-adjacent vertices. The first and second Zagreb co-indices were first introduced by Došlić [9]. They are defined as follows:

$$\bar{M_1}(G) = \sum_{uv \notin E(G)} [deg(u) + deg(v)],$$

$$\bar{M_2}(G) = \sum_{uv \notin E(G)} [deg(u)deg(v)].$$

In [3], the authors considered some mathematical properties of this new graph invariant.

The eccentricity $\varepsilon_G(u)$ is the largest distance between u and any other vertex v of G. We will omit the subscript G when the graph is clear from the context. The eccentric connectivity index of G is defined as $\xi^c(G) = \sum_{u \in V(G)} \varepsilon(u)deg(u)$ [20].

We encourage the reader to consult papers [1, 2, 21] for some applications and [10, 15, 25] for the mathematical properties of this topological index.

In this article we study graph invariants, the first Zagreb index and co-index, Wiener index and eccentric connectivity index under hierarchical product of graphs [4]. One of us (ARA) in some earlier papers considered the same problem for other graph operations, see [3, 14, 16, 17, 18, 24] for details. Throughout this paper our notation is standard. The complete graph and path on n vertices are denoted by K_n and P_n, respectively. For terms and concepts not defined here we refer the reader to any of several standard monographs such as, e.g., [8] or [22].

2. Main Results. In this section exact formulas for some graph invariants under the hierarchical product of graphs are obtained. The hierarchical product is a new graph operation introduced by Barrière et al. [4]. Following Barrière et al. [5], the binary hypertree of dimension m is defined as the hierarchical product of m copies of the complete graph K_2. Since the graphs obtained from the hierarchical product are spanning subgraphs of the corresponding Cartesian products, we obtain that the binary hypertree of dimension m is a spanning subgraph of the hypercube Q_m. Then the authors applied this fact to obtain some nice results on this class of trees. We refer the interested readers to [6, 7] for a generalization of this concept and some other mathematical properties of hierarchical product.

Let G_1 and G_2 be graphs with vertex sets V_1 and V_2, respectively, having a distinguished or root vertex, labeled 0. The hierarchical product $H = G_2 \sqcap G_1$ is the graph with vertices the tuples x_2x_1, $x_i \in V_i$, $i = 1, 2$, and edges defined as follows:

$$x_2x_1 \sim \begin{cases} x_2y_1, & \text{if } y_1x_1 \in E(G_1), \\ y_2x_1, & \text{if } y_2x_2 \in E(G_2) \text{ and } x_1 = 0. \end{cases}$$

Notice that the structure of the obtained product graph H heavily depends on the root vertices of the factors G_1 and G_2.

Theorem 1. *Suppose G_1 and G_2 are connected graphs with vertex sets V_1 and V_2, respectively. Then* $W(G_2 \sqcap G_1) = |V_2|W(G_1) + |V_1|^2W(G_2) + (|V_2|^2 - |V_2|)|V_1|D_{G_1}(0)$, *where $D_{G_1}(0)$ denotes the summation of all distances between 0 and other vertices of G_1.*

P r o o f. Suppose $x = x_2x_1, y = y_2y_1 \in V(G_2 \sqcap G_1)$, where $x_1, y_1 \in V_1$ and $x_2, y_2 \in V_2$. Apply [4, Proposition 2.4], we have:

$$\begin{aligned} W(G_2 \sqcap G_1) &= \sum_{\{x,y\} \in V(G_2 \sqcap G_1)} d_{G_2 \sqcap G_1}(x,y) \\ &= \sum_{\substack{\{x_1,y_1\} \in V_1 \\ x_2,y_2 \in V_2; x_2 = y_2}} d_{G_1}(x_1,y_1) \\ &+ \sum_{\substack{\{x_1,y_1\} \in V_1 \\ x_2,y_2 \in V_2; x_2 \neq y_2}} (d_{G_2}(x_2,y_2) + d_{G_1}(x_1,0) + d_{G_1}(0,y_1)) \\ &= |V_2|W(G_1) + |V_1|^2 W(G_2) + (|V_2|^2 - |V_2|)|V_1| D_{G_1}(0), \end{aligned}$$

which completes our argument. □

Corollary 2. *Suppose G is a connected graph. Then the Wiener index of $P_n \sqcap G$ and alkanes $P_n \sqcap P_n$ are computed as follows:*

$$\begin{aligned} W(P_n \sqcap G) &= nW(G) + |V(G)|^2 \frac{n(n^2-1)}{6} + (n^2 - n)|V(G)| D_G(0), \\ W(P_n \sqcap P_n) &= (n^3 + n^2)\frac{(n^2-1)}{6} + n^2(n-1)D_G(0). \end{aligned}$$

Theorem 3. *Suppose G_1 and G_2 are connected graphs. Then $\xi^c(G_2 \sqcap G_1) = (\delta_1 + \delta_2)(\varepsilon_2 + \varepsilon_1) + (\delta_1|V(G_1)| + \delta_2)(\zeta(G_2) - \varepsilon_2) + (|V(G_2)| - 1)(\delta_1 + \delta_2)\varepsilon_1 + \delta_1|V(G_2)|D_{G_1}(0) + |V(G_2)|(|V(G_1)| - 1)\delta_1\varepsilon_1 + \delta_1\varepsilon_2(|V(G_1)| - 1)$, where $\zeta(G) = \sum_{v \in V(G)} \varepsilon(v)$ is called the total eccentricity of G.*

P r o o f. Suppose $x = x_2x_1 \in V(G_2 \sqcap G_1)$ and δ_i and ε_i, $i = 1, 2$, are the degree and eccentricity of root vertex of G_i, respectively. Applying [4, Proposition 2.4] and the definition of hierarchical product of graphs, we have:

$$\xi^c(G_2 \sqcap G_1) = \sum_{x \in V(G_2 \sqcap G_1)} \varepsilon_{V(G_2 \sqcap G_1)}(x) deg_{V(G_2 \sqcap G_1)}(x)$$

$$
\begin{aligned}
&= (\delta_1+\delta_2)(\varepsilon_2+\varepsilon_1) + \sum_{x=x_2 0; x_2\in V(G_2)} (\delta_1+\delta_2)(\varepsilon_{G_2}(x_2)+\varepsilon_1)\\
&+ \sum_{\substack{x=x_2x_1\\ x_1\neq 0\in V(G_1); x_2\in V(G_2)}} \delta_1(\varepsilon_{G_2}(x_2)+d_{G_1}(x_1,0)+\varepsilon_1)\\
&= (\delta_1+\delta_2)(\varepsilon_2+\varepsilon_1) + (\delta_1+\delta_2)\sum_{x_2\neq 0\in V(G_2)} \varepsilon_{G_2}(x_2)\\
&+ (|V(G_2)|-1)(\delta_1+\delta_2)\varepsilon_1 + \delta_1(|V(G_1)|-1)\sum_{x_2\neq 0\in V(G_2)} \varepsilon_{G_2}(x_2)\\
&+ \delta_1|V(G_2)|D_{G_1}(0) + |V(G_2)|(|V(G_1)|-1)\delta_1\varepsilon_1 + \delta_1\varepsilon_2(|V(G_1)|-1)\\
&= (\delta_1+\delta_2)(\varepsilon_2+\varepsilon_1) + (\delta_1|V(G_1)|+\delta_2)(\zeta(G_2)-\varepsilon_2)\\
&+ (|V(G_2)|-1)(\delta_1+\delta_2)\varepsilon_1 + \delta_1|V(G_2)|D_{G_1}(0)\\
&+ |V(G_2)|(|V(G_1)|-1)\delta_1\varepsilon_1 + \delta_1\varepsilon_2(|V(G_1)|-1),
\end{aligned}
$$

which completes our argument. □

Corollary 4. *Suppose G_1 is a connected graph, and δ_1 and ε_1 are the degree and eccentricity of the root vertex of G_1, respectively. Then the eccentric connectivity index of $P_n \sqcap G_1$ and alkanes $P_n \sqcap P_n$ are computed as follows:*

1) *If n is even then:*

$$
\begin{aligned}
\xi^c(P_n\sqcap G_1) &= (\delta_1+\delta_{P_n})(\varepsilon_1+\varepsilon_{P_n}) + (\delta_1|V(G_1)|+\delta_{P_n})\left(\frac{3n^2+2n}{4}-\varepsilon_{P_n}\right)\\
&\quad +(n-1)(\delta_1+\delta_{P_n})\varepsilon_1 + n\delta_1 D_{G_1}(0) + n(|V(G_1)|-1)\delta_1\varepsilon_1\\
&\quad +\delta_1\varepsilon_{P_n}(|V(G_1)|-1),\\
\xi^c(P_n\sqcap P_n) &= 4\delta_{P_n}\varepsilon_{P_n} + \delta_{P_n}(n+1)\left(\frac{3n^2+2n}{4}-\varepsilon_{P_n}\right) + 2(n-1)\delta_{P_n}\varepsilon_{P_n}\\
&\quad +n\delta_{P_n}D_{P_n}(0) + n(n-1)\delta_{P_n}\varepsilon_{P_n} + \delta_{P_n}\varepsilon_{P_n}(n-1).
\end{aligned}
$$

2) *If n is odd then:*

$$\begin{aligned}\xi^c(P_n \sqcap G_1) &= (\delta_1+\delta_{P_n})(\varepsilon_1+\varepsilon_{P_n}) + (n-1)(\delta_1+\delta_{P_n})\varepsilon_1 + n\delta_1 D_G(0)\\ &\quad +(\delta_1|V(G_1)|+\delta_{P_n})\left(\frac{3}{4}(n^2-1)+\frac{n-1}{2}-\varepsilon_{P_n}\right)\\ &\quad +n(|V(G_1)|-1)\delta_1\varepsilon_1 + \delta_1\varepsilon_{P_n}(|V(G_1)|-1),\\ \xi^c(P_n \sqcap P_n) &= \delta_{P_n}(n+1)\left(\frac{3}{4}(n^2-1)+\frac{n-1}{2}-\varepsilon_{P_n}\right) + 2(n+1)\delta_{P_n}\varepsilon_{P_n}\\ &\quad +n\delta_{P_n}D_{P_n}(0) + n(n-1)\delta_{P_n}\varepsilon_{P_n} + \delta_{P_n}\varepsilon_{P_n}(n-1).\end{aligned}$$

In the following theorem, we use the notations given in the proof of Theorem 3.

Theorem 5. *Suppose G_1 and G_2 are connected graphs. Then the first Zagreb index of the hierarchical product is computed as follows:*

$$M_1(G_2 \sqcap G_1) = |V(G_2)||V(G_1)|{\delta_1}^2 + |V(G_2)|{\delta_2}^2 + 2|V(G_2)|\delta_1\delta_2.$$

P r o o f. Suppose $H = G_2 \sqcap G_1$ and $x = x_2x_1 \in V(H)$. Consider three separate cases for x and apply [4, Equation 5]. If $x = 00$ then $\deg_H(x) = \delta_1 + \delta_2$. If $x = x_20$, $x_2 \neq 0$, then there are $|V(G_2)| - 1$ choices for the vertex x_2 and $\deg_H(x) = \delta_1 + \delta_2$. Finally, if $x = x_2x_1$, $x_1 \neq 0$, then there are $|V(G_1)| - 1$ choices for the vertex x_1, $|V(G_2)|$ choices for x_2 and $\deg_H(x) = \delta_1$.

$$\begin{aligned}M_1(G_2 \sqcap G_1) &= \sum_{v\in V(G_2\sqcap G_1)} deg^2_{G_2\sqcap G_1}(v)\\ &= (|V(G_2)|-1)(\delta_1+\delta_2)^2 + |V(G_2)|(|V(G_1)|-1){\delta_1}^2 + (\delta_1+\delta_2)^2\\ &= |V(G_2)||V(G_1)|{\delta_1}^2 + |V(G_2)|{\delta_2}^2 + 2|V(G_2)|\delta_1\delta_2,\end{aligned}$$

which completes our argument. □

Corollary 6. *With the notations of Theorem 3, we have:*

$$a)\ M_1(P_n \sqcap G_1) = n|V(G_1)|{\delta_1}^2 + n{\delta_{P_n}}^2 + 2n\delta_1\delta_{P_n},$$

$$\begin{aligned}
b)\ M_1(P_n \sqcap P_n) &= {\delta_{P_n}}^2(n^2+3n),\\
c)\ \bar{M}_1(G_2 \sqcap G_1) &= 2|E(G_2 \sqcap G_1)|(|V(G_2 \sqcap G_1)|-1) - M_1(G_2 \sqcap G_1)\\
&= 2(|E(G_2)| + |V(G_2)||E(G_1)|)(|V(G_1)||V(G_2)|-1)\\
&\quad -M_1(G_2 \sqcap G_1),\\
d)\ \bar{M}_1(P_n \sqcap G_1) &= 2(n-1+n|E(G_1)|)(|V(G_1)|n-1) - M_1(P_n \sqcap G_1),\\
e)\ \bar{M}_1(P_n \sqcap P_n) &= 2(n-1)^2 - {\delta_{P_n}}^2(n^2+3n),\\
f)\ M_2(P_n \sqcap G_1) &= (n-1)(\delta_1+1)^2 + n(M_2(G_1)+{\delta_1}^2),\\
g)\ M_2(P_n \sqcap P_n) &= (n-1)(\delta_{P_n}+1)^2 + n(4n-8+{\delta_{P_n}}^2),\\
h)\ \bar{M}_2(P_n \sqcap G_1) &= 2(n-1+n|E(G_1)|)^2 - (n-1)(\delta_1+1)^2\\
&\quad -n(M_2(G_1)+{\delta_1}^2) - \frac{1}{2}(n|V(G_1)|{\delta_1}^2 + n{\delta_{P_n}}^2 + 2n\delta_1\delta_{P_n}),\\
i)\ \bar{M}_2(P_n \sqcap P_n) &= 2(n-1+n(n-1))^2 - (n-1)(\delta_{P_n}+1)^2\\
&\quad -n(4n-8+{\delta_{P_n}}^2) - \frac{1}{2}{\delta_{P_n}}^2(n^2+3n).
\end{aligned}$$

Proof. Apply Theorem 5 and [3, Propositions 2 and 4]. □

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REFERENCES

[1] Ashrafi A. R., M. Saheli, M. Ghorbani. The eccentric connectivity index of nanotubes and nanotori. *J. Comput. Appl. Math.*, **235** (2011), 4561–4566.

[2] Ashrafi A. R., T. Došlić, M. Saheli. The eccentric connectivity index of $TUC_4C_8(R)$ nanotubes. *MATCH Commun. Math. Comput. Chem.,* **65** (2011), No 1, 221–230.

[3] Ashrafi A. R., T. Došlić, A. Hamzeh. The Zagreb coindices of graph operations. *Discrete Appl. Math.,* **158**(2010), No 15, 1571–1578.

[4] Barrière L., F. Comellas, C. Dalfó, M. A. Fiol. The hierarchical product of graphs. *Discrete Appl. Math.,* **157** (2009), No 1, 36–48.

[5] Barrière L., F. Comellas, C. Dalfó, M. A. Fiol. On the spectra of hypertrees, *Linear Algebra Appl.,* **428** (2008), No 7, 1499–1510.

[6] Barrière L., F. Comellas, C. Dalfó, M. A. Fiol. On the hierarchy product of graphs and the generalized binomial tree. *Linear Multilinear Algebra*, **57** (2009), No 7, 695–712.

[7] Barrière L., C. Dalfó, M. A. Fiol, M. Mitjana. The generalized hierarchical product of graphs. *Discrete Math.,* **309** (2009), No 12, 3871–3881.

[8] Diudea M. V., I. Gutman, L. Jantschi. Molecular Topology. Huntington, NY, 2001.

[9] Došlić T. Vertex-weighted Wiener polynomials for composite graphs. *Ars Math. Contemp.,* **1** (2008), No 1, 66–80.

[10] Došlić T., M. Saheli, D. Vukicevic. Eccentric connectivity index: extremal graphs and values. *Iranian J. Math. Chem.,* **1** (2010), No 2, 45–56.

[11] Guo Y., Y. Du, Y. Wang. Bipartite graphs with extreme values of the first general Zagreb index. *MATCH Commun. Math. Comput. Chem.,* **63** (2010), No 2, 469–480.

[12] Gutman I., K. Ch. Das. The first Zagreb index 30 years after. *MATCH Commun. Math. Comput. Chem.,* **50** (2004), 83–92.

[13] Gutman I., N. Trinajstic. Graph theory and molecular orbitals. Total $\pi-$electron energy of alternant hydrocarbons. *Chem. Phys. Lett.,* **17** (1972), 535–538.

[14] Hossein-Zadeh S., A. Hamzeh, A. R. Ashrafi. Wiener-type invariants of some graph operations. *FILOMAT*, **29** (2009), No 3, 103–113.

[15] Ilić A., I. Gutman. Eccentric connectivity index of chemical trees. *MATCH Commun. Math. Comput. Chem.,* **65** (2011), No 3, 731–744.

[16] Khalifeh M. H., H. Yousefi-Azari, A. R. Ashrafi. The first and second Zagreb indices of graph operations. *Discrete Appl. Math.,* **157** (2009), No 4, 804–811.

[17] Khalifeh M. H., H. Yousefi-Azari, A.R. Ashrafi. The hyper-Wiener index of graph operations. *Comput. Math. Appl.,* **56** (2008), No 5, 1402–1407.

[18] Khalifeh M. H., H. Yousefi-Azari, A. R. Ashrafi. A matrix method for computing Szeged and vertex PI indices of join and composition of graphs. *Linear Algebra Appl.,* **429**(2008), No 11-12, 2702–2709.

[19] Nikolić S., G. Kovačević, A. Miličević, N. Trinajstić. The Zagreb indices 30 years after. *Croat. Chem. Acta,* **76** (2003), No 2, 113–124.

[20] Sharma V., R. Goswami, A. K. Madan. Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies. *J. Chem. Inf. Comput. Sci.,* **37** (1997), 273–282.

[21] Sardana S., A. K. Madan. Application of graph theory: Relationship of molecular connectivity index, Wiener's index and eccentric connectivity index with diuretic activity. *MATCH Commun. Math. Comput. Chem.,* **43** (2001), 85–98.

[22] West D. B. Introduction to Graph Theory. Prentice Hall, Upper Saddle River, USA, 1996.

[23] Wiener, H. Structural determination of the paraffin boiling points. *J. Am. Chem. Soc.,* **69** (1947), 17–20.

[24] Yousefi-Azari H., B. Manoochehrian, A. R. Ashrafi. The PI index of product graphs. *Appl. Math. Lett.,* **21** (2008), No 6, 624–627.

[25] Zhou B., Z. Du. On eccentric connectivity index. *MATCH Commun. Math. Comput. Chem.,* **63** (2010), No 1, 181–198.

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