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Zagreb Indices of the Generalized Hierarchical Product of Graphs

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Abstract. In this paper the first and the second Zagreb indices of generalized hierarchical product of graphs, which is generalization of standard hierarchical and Cartesian product of graphs, is computed. As a consequence we compute the Zagreb indices of some chemical graphs.

1 Introduction

In the early work of the Zagreb mathematical chemistry group on the topological basis of π-electron energy, in 1972, two terms appeared in the approximate formula for the π-energy of conjugated molecules [1]-[2], which were later used separately as topological indices in QSPR and QSAR studies [3]-[4].

Let $G = (V(G), E(G)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Then the first and second Zagreb indices are defined as

$$M_1(G) = \sum_{v \in V(G)} \delta(v)^2$$

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

where $\delta(v)$ is the degree of vertex v (see [1]). We encourage the reader to consult [5]-[10] for historical background, computational techniques and mathematical properties of Zagreb indices.

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A new operation on graphs, namely hierarchical product, were introduced by Spain mathematicians, L. Barriere and coauthors in 2009 (see [11]). Also a generalization of both Cartesian and the hierarchical product of graphs, namely generalization hierarchical product of graphs, were reported by this team in 2009 (see [12]).

Now we recall these graph operations. Let $G = (V(G), E(G))$ and $H = (V(H), E(H))$ be two graphs and U be a non-empty subset of $V(H)$. Let $\Gamma = G \sqcap H(U)$ be the hierarchical product of G and H corresponding to U. Then $V(\Gamma) = V(G) \times V(H)$ and $(a, x)(b, y) \in E(\Gamma)$ if and only if $a = b, xy \in E(H)$ or $ab \in E(G), x = y \in U$. It is clear that if $U = V(H)$, then $G \sqcap H(U) = G \square H$, the Caretesian product of G and H. Also if $U = \{z\}$ be a singleton, then $G \sqcap H(U) = G \sqcap H$, the (standard) hierarchical product of G and H with root vertex z. The hierarchical product can be naturally extended for more than two graphs (see [11]).

Note that the structure of the generalized hierarchical product Γ heavily depends on the subset U of $V(H)$. Note also that Γ is simply a subgraph of the classical Cartesian product of G and H. Although the Cartesian product is both commutative and associative, the generalized hierarchical product has only the second property, provided that the subsets are conveniently chosen. Moreover such a product is also distributive on the right with respect to the union of graphs.

Through this paper our notation is standard and taken mainly from [13]. P_n, C_n and K_n are a path, a cycle and a complete graph on n vertices, respectively. By simple calculations one can see that $M_1(P_n) = 4n - 6$, $M_2(P_n) = 4n - 8$ for $n \geq 3$. Moreover $M_1(P_1) = 0$, $M_1(P_2) = 2$, $M_2(P_1) = 0$ and $M_2(P_2) = 1$. Also $M_1(C_n) = M_2(C_n) = 4n$, $M_1(K_n) = n(n-1)^2$ and $M_2(K_n) = \frac{n(n-1)^3}{2}$.

2 Main Results

In this section, some exact formulae for the first and second Zagreb indices of the generalized hierarchical product of graphs are presented. We begin with the following crucial lemma related to the degree of a vertex in generalized hierarchical product of graphs.

Lemma 2.1. (see [12]) The degree of a vertex $x = (x_N, x_{N-1}, \ldots, x_2, x_1)$ in the generalized hierarchical product $H_N = G_N \sqcap \cdots \sqcap G_2(U_2) \sqcap G_1(U_1)$ is

$$\delta(x) = \delta(x_1) + \chi_{U_1}(x_1)\delta(x_2) + \cdots + \left[\chi_{U_1}(x_1) \cdots \chi_{U_{N-1}}(x_{N-1})\right] \delta(x_N)\,,$$

where δ and χ_{U_i} denote, respectively, the degree and the characteristic function on the set U_i which is 1 on U_i and 0 outside U_i.

Theorem 1. Let $\Gamma = G \sqcap H(U)$. Then

$$M_1(\Gamma) = |V(G)|M_1(H) + |U|M_1(G) + 4|E(G)|\sum_{u\in U}\delta(u)\ .$$

Proof. For every $v = (g,h) \in V(\Gamma)$, we have $\delta(v) = \delta(h) + \chi_U(h)\delta(g)$. Thus

$$\begin{aligned} M_1(\Gamma) &= \sum_{v\in V(\Gamma)}\delta(v)^2 = \sum_{g\in V(G),h\in V(H)}(\delta(h)+\chi_U(h)\delta(g))^2 \\ &= |V(G)|\sum_{h\in V(H)}\delta(h)^2 + |U|\sum_{g\in V(G)}\delta(g)^2 + 2\sum_{g\in V(G),u\in U}\delta(g)\delta(u) \\ &= |V(G)|M_1(H) + |U|M_1(G) + 2\sum_{g\in V(G)}\delta(g)\sum_{u\in U}\delta(u) \\ &= |V(G)|M_1(H) + |U|M_1(G) + 4|E(G)|\sum_{u\in U}\delta(u) \end{aligned}$$

as desired. ■

We know that if $U = V(H)$, then $G \sqcap H(U) = G\Box H$ and if U is a singleton, then $G \sqcap H(U) = G \sqcap H$. So we have the following corollary:

Corollary 2.2. Let $G = (V(G), E(G))$ and $H = (V(H), E(H))$ be two graphs. Then
(a)If $G\Box H$ is the Cartesian product of G and H, then

$$M_1(G\Box H) = |V(G)|M_1(H) + |V(H)|M_1(G) + 8|E(G)||E(H)|$$

(b) If $G \sqcap H$ is the standard hierarchical product of G and H with root vertex z, then

$$M_1(G \sqcap H) = |V(G)|M_1(H) + M_1(G) + 4|E(G)|\delta(z)\ .$$

■

If for $j > k$, we put $\sum_{i=j}^{k} f(i) = 0$ and $\prod_{i=j}^{k} f(i) = 1$, then we can simplify the first Zagreb index of generalized hierarchical product of N graphs as follows:

Corollary 2.3. Let $G_i = (V_i, E_i)$, $U_i \subseteq V_i$ and $H_N = G_N \sqcap G_{N-1}(U_{N-1}) \sqcap \cdots \sqcap G_1(U_1)$, $N \geq 2$. Then

$$\begin{aligned} M_1(H_N) &= \sum_{i=1}^{N}\left[M_1(G_i)\prod_{j=1}^{i-1}|U_j|\prod_{k=i+1}^{N}|V_k|\right] \\ &+ 4\sum_{i=1}^{N-1}\left[\sum_{u\in U_i}\delta(u)\left(\sum_{j=i+1}^{N}[|E_j|\prod_{k=1,k\neq i}^{j-1}|U_k|\prod_{r=j+1}^{N}|V_r|]\right)\right]\ . \end{aligned}$$

Proof. By associativity of generalized hierarchical product and lemma 1 and inductive argument, we have

$$\begin{aligned}
M_1(H_{N+1}) &= M_1(G_{N+1} \sqcap H_N(U_N \times \cdots \times U_1)) \\
&= |V_{N+1}| M_1(H_N) + M_1(G_{N+1}) \prod_{i=1}^{N} |U_i| + 4|E_{N+1}| \sum_{u=(u_N,\ldots,u_1)\in U_N\times\cdots\times U_1} \delta(u) \\
&= |V_{N+1}| \left(\sum_{i=1}^{N} \left[M_1(G_i) \prod_{j=1}^{i-1} |U_j| \prod_{k=i+1}^{N} |V_k| \right] \right. \\
&+ \left. 4 \sum_{i=1}^{N-1} \left[\sum_{u\in U_i} \delta(u) \left(\sum_{j=i+1}^{N} [|E_j| \prod_{k=1,k\neq i}^{j-1} |U_k| \prod_{r=j+1}^{N} |V_r|] \right) \right] \right) \\
&+ M_1(G_{N+1}) \prod_{i=1}^{N} |U_i| + 4|E_{N+1}| \left(\sum_{i=1}^{N} \left[\prod_{j=1,j\neq i}^{N} |U_j| \sum_{u\in U_i} \delta(u) \right] \right) \\
&= \sum_{i=1}^{N+1} \left[M_1(G_i) \prod_{j=1}^{i-1} |U_j| \prod_{k=i+1}^{N} |V_k| \right] \\
&+ 4 \sum_{i=1}^{N} \left[\sum_{u\in U_i} \delta(u) \left(\sum_{j=i+1}^{N+1} \left[|E_j| \prod_{k=1,k\neq i}^{j-1} |U_k| \prod_{r=j+1}^{N+1} |V_r| \right] \right) \right]
\end{aligned}$$

as desired. ■

Corollary 2.4. Let $G_i = (V_i, E_i)$ be a graph for $1 \leq i \leq n$ with root vertex z_i. Then

$$M_1(G_n \square \cdots \square G_1) = |V| \left(\sum_{i=1}^{n} \frac{M_1(G_i)}{|V_i|} + 8 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{|E_i||E_j|}{|V_i||V_j|} \right)$$

$$M_1(G_n \sqcap \cdots \sqcap G_1) = \sum_{i=1}^{n} \left[M_1(G_i) \prod_{j=i+1}^{n} |V_j| \right] + 4 \sum_{i=1}^{n-1} \left[\delta(z_i) \sum_{j=i+1}^{n} |E_j| \prod_{k=j+1}^{n} |V_k| \right] .$$

In particular if $G_1 = G_2 = \cdots = G_n = G$ where $G = (V, E)$ is a graph with root vertex z, and $G^n = G \square \cdots \square G$ (n-times) and $G^{[n]} = G \sqcap \cdots \sqcap G$ (n-times), then

$$M_1(G^n) = n|V|^{n-2} \left(|V| M_1(G) + 4|E|^2 (n-1) \right)$$

and

$$M_1(G^{[n]}) = \frac{(|V|^n - 1)(|V| - 1) M_1(G) + 4|E|\delta(z)(|V|^n - n|V| + n - 1)}{(|V| - 1)^2} .$$

Now we give an important lemma as follows.

Lemma 2.5. Let $G = (V(G), E(G))$ be a r-regular graph. Then $M_1(G) = |V(G)|r^2$ and $M_2(G) = |E(G)|r^2 = \frac{r^3|V(G)|}{2}$.

Proof. Since in any r-regular graph the degree of any vertex is r, and $\sum_{v\in V(G)} \delta(v) = 2|E(G)|$, the result is clear. ■

Let G be a molecular graph of a fullerene with n vertices. Since G is a 3-regular graph, $M_1(G) = 9n$ and $M_2(G) = \frac{27n}{2}$. For example $M_1(C_{60}) = 540$ and $M_2(C_{60}) = 810$.

Corollary 2.6. Let G and H be r and s-regular graphs, respectively. Then

$$M_1(G\Box H) = |V(G)||V(H)|(s+r)^2\,, \tag{1}$$

$$M_1(G \sqcap H) = |V(G)|(s^2|V(H)| + 2rs + r^2) \tag{2}$$

and more generally, if $G_1, \ldots, G_n$ be $r_1, \ldots, r_n$-regular graphs, respectively, then

$$M_1(G_1\Box G_2\Box\cdots\Box G_n) = |V_1||V_2|\cdots|V_n|(r_1+r_2+\cdots+r_n)^2\,, \tag{3}$$

$$M_1(G_n \sqcap \cdots \sqcap G_2 \sqcap G_1) = \sum_{i=1}^{n}\prod_{j=i}^{n} r_i^2|V_j| + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\prod_{k=j}^{n} r_ir_j|V_k| \tag{4}$$

where $|V_i|$ is the number of all vertices of G_i. In particular if G be a r-regular graph, then

$$M_1(G^n) = |V(G)|^n n^2 r^2$$

and

$$M_1(G^{[n]}) = \frac{r^2|V(G)|\left(|V(G)|^{n+1} + |V(G)|^n - |V(G)|(1+2n) + 2n - 1\right)}{(|V(G)|-1)^2}\,.$$

Using the above corollary we can give the following examples.

Example 2.7. Let $G = C_{n_1} \otimes C_{n_2} \otimes \cdots \otimes C_{n_k}$, $k \geq 2$, be a tori graph. Then $M_1(G) = 4n_1n_2\cdots n_k k^2$. If $k = 2$, then the resulting graph is a C_4-tori and in this case $M_1(C_{n_1} \otimes C_{n_2}) = 16n_1n_2$.

Example 2.8. Let $G = K_{n_1} \otimes K_{n_2} \otimes \cdots \otimes K_{n_r}$. Since K_{n_i} is a $n_i - 1$-regular graph, so $M_1(G) = n_1n_2\cdots n_r(n_1 + n_2 + \cdots + n_r - r)^2$.

As a corollary we can compute the first zagreb index of a hypercube of dimension n, Q_n. We know that $Q_n = \bigotimes_{i=1}^{n} K_2$, where K_2 is the complete graph on 2 vertices. K_2 is a 1-regular graph. So $M_1(Q_n) = 2^n n^2$. It is well-known fact that a graph G is a

Hamming graph if and only if it can be written in the form $G = \bigotimes_{i=1}^{r} K_{n_i}$ where K_{n_i} is the complete graph on n_i vertices and so the Hamming graph G is usually denoted as $H_{n_1,\ldots,n_r}$. So $M_1(H_{n_1,\ldots,n_r}) = n_1 n_2 \cdots n_r (n_1 + n_2 + \cdots + n_r - r)^2$.

Example 2.9. Consider the binary hypertree T_m which is the standard hierarchical product of m copies of the complete graph K_2. So $T_m = K_2^{[m]}$ and $M_1(T_m) = 3 \cdot 2^{m+1} - 4m - 6$.

Now we give an exact formula for the second Zagreb index of generalized hierarchical product of graphs.

If for every $x \in V(G)$, we define $N[x]$ as the set of all adjacent vertices of x, then we have

Theorem 2. Let $\Gamma = G \sqcap H(U)$. Then

$$\begin{aligned} M_2(\Gamma) &= |V(G)|M_2(H) + |U|M_2(G) + 2|E(G)| \sum_{u\in U} \sum_{x\in N[u]} \delta(x) \\ &+ M_1(G)\,|\{xy \in E(H) \mid x, y \in U\}| + |E(G)| \sum_{u\in U} \delta(u)^2 + M_1(G) \sum_{u\in U} \delta(u) \end{aligned}$$

Proof. Since $E(\Gamma) = \{(a,x)(a,y) \mid a \in V(G), xy \in E(H)\} \cup \{(a,x)(b,x) \mid ab \in E(G), x \in U\}$, we have

$$\begin{aligned} M_2(\Gamma) &= \sum_{a\in V(G), xy\in E(H)} \delta(a,x)\delta(a,y) + \sum_{ab\in E(G), x\in U} \delta(a,x)\delta(b,x) \\ &= \sum_{a\in V(G), xy\in E(H)} (\delta(x) + \chi_U(x)\delta(a))\,(\delta(y) + \chi_U(y)\delta(a)) \\ &+ \sum_{ab\in E(G), x\in U} (\delta(x) + \delta(a))\,(\delta(x) + \delta(b)) \ . \end{aligned}$$

By a simple calculation one can see that

$$\begin{aligned} &\sum_{a\in V(G), xy\in E(H)} (\delta(x) + \chi_U(x)\delta(a))\,(\delta(y) + \chi_U(y)\delta(a)) \\ &= |V(G)|M_2(H) + 2|E(G)| \left(\sum_{xy\in E(H), y\in U} \delta(x) + \sum_{xy\in E(H), x\in U} \delta(y) \right) \\ &+ M_1(G) \mid \{xy \in E(H) \mid x, y \in U\} \mid \\ &= |V(G)|M_2(H) + 2|E(G)| \sum_{u\in U} \sum_{x\in N[u]} \delta(x) + M_1(G) \mid \{xy \in E(H) \mid x, y \in U\} \mid \end{aligned}$$

and

$$\sum_{ab\in E(G),x\in U}(\delta(x)+\delta(a))(\delta(x)+\delta(b))=|E(G)|\sum_{x\in U}\delta(x)^2+M_1(G)\sum_{x\in U}\delta(x)+|U|M_2(G)\ .$$

Note that in the last equality we used this fact that $\sum_{ab\in E(G)}[\delta(a)+\delta(b)]=M_1(G)$. Now the result is clear. ■

If we put $U=V(H)$ or $U=\{z\}$, then we have the following corollary:

Corollary 2.10. Let $G\Box H$ and $G\sqcap H$ be the Cartesian and standard hierarchical product of G and H with root vertex z, respectively. Then

$$\begin{aligned} M_2(G\Box H) &= |V(G)|M_2(H)+|V(H)|M_2(G)+3|E(H)|M_1(G)+3|E(G)|M_1(H) \\ M_2(G\sqcap H) &= |V(G)|M_2(H)+M_2(G)+2|E(G)|\sum_{x\in N[z]}\delta(x) \\ &+ |E(G)|\delta(z)^2+M_1(G)\delta(z) \end{aligned}$$

■

Corollary 2.11. If G and H be r and s-regular graphs, respectively, then

$$\begin{aligned} M_2(G\Box H) &= \frac{1}{2}|V(G)||V(H)|(s+r)^3 \\ M_2(G\sqcap H) &= \frac{|V(G)|}{2}\left(s^3|V(H)|+r^3+2rs|N[z]|+rs^2+2r^2s\right)\ . \end{aligned}$$

Inductively one can see that if G_i be a r_i-regular graph for every $1\le i\le n$, then

$$M_2(G_1\Box\cdots\Box G_n)=\frac{1}{2}|V_1|\cdots|V_n|(r_1+\cdots+r_n)^3\ .$$

As a corollary, we have

$$M_2(C_{n_1}\Box\cdots\Box C_{n_k})=4n_1\cdots n_k k^3$$

$$M_2(K_{n_1}\Box\cdots\Box K_{n_r})=\frac{1}{2}n_1\cdots n_r(n_1+\cdots+n_r-r)^3\ .$$

Now we consider some chemical structures and compute the first and second Zagreb indices of these structures.

Let $\Gamma=P_2\sqcap H(U)$, then by Theorem 1, $M_1(\Gamma)=2M_1(H)+2|U|+4\sum_{u\in U}\delta(u)$ and by Theorem 2,

$$\begin{aligned} M_2(\Gamma) &= 2M_2(H)+|U|+2\sum_{u\in U}\sum_{x\in N[u]}\delta(x)+2\left|\{xy\in E(H)\mid x,y\in U\}\right| \\ &+ 2\sum_{u\in U}\delta(u)^2+2\sum_{u\in U}\delta(u)\ . \end{aligned}$$

Now we consider some chemical structures of the form $P_2 \sqcap H(U)$ and compute the first and second Zagreb indices of them.

Example 2.12. Let $\Gamma = DD_{p,r} = P_2 \sqcap H$ (see Figure 1). Then $M_1(\Gamma) = 2M_1(H) + 2 + 4p$. But $M_1(H) = \frac{p(p^{r+1}+3p^r-3p-1)}{p-1}$. So $M_1(\Gamma) = \frac{2(p^{r+2}+3p^{r+1}-p^2-2p-1)}{p-1}$. Also $M_2(P_2 \sqcap H) = 2M_2(H) + 3p^2 + 4p + 1$. But $M_2(H) = \frac{2p(1+p)(p^r-p)}{p-1}$ and so $M_2(\Gamma) = \frac{(1+p)(4p^{r+1}-p^2-2p-1)}{p-1}$.

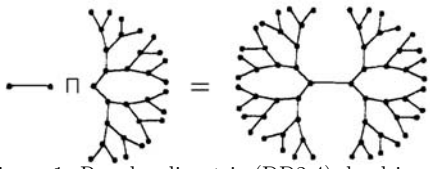

Figure 1: Regular dicentric (DD2.4) dendrimer.

Example 2.13. Consider the molecular graph of linear phenelyne F_n including n benzene rings (see Figure 2). Then $F_n = P_2 \sqcap P_{3n}(U)$ where $U = \{1, 4, 7, .., 3n-2\} \cup \{3, 6, 9, ..., 3n\}$. It is easy to see that $M_1(F_n) = 44n - 20$. $M_2(F_n) = 60n - 40$.

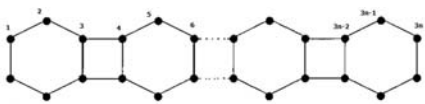

Figure 2: A linear phenylene

Example 2.14. Let n be an even positive integer number and R_n be a cyclic phenelyne including n benzene ring (see Figure 3). Then $R_n = P_2 \sqcap F_{\frac{n}{2}}$. So $M_1(R_n) = 44n$ and $M_2(R_n) = 60n - 4$.

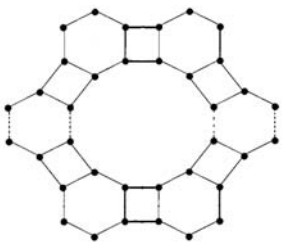

Figure 3: A cyclic phenylene

Example 2.15. Let $\Gamma = P_2 \sqcap C_{60}(U)$ be the molecular graph of dimer fullerene (see Figure 4). Then $M_1(\Gamma) = 1108$ and $M_2(\Gamma) = 1674$.

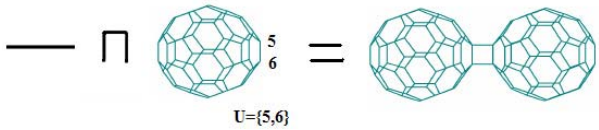

Figure 4: Dimer fullerene C_{60}

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